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SOLUBILITY DATA SERIES

Volume 54

POLYCYCLIC AROMATIC HYDROCARBONS IN PURE AND BINARY SOLVENTS

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Volume 54

POLYCYCLIC AROMATIC HYDROCARBONS IN PURE AND BINARY SOLVENTS

Volume Editor

WILLIAM E. ACREE, Jr.

University of North Texas
Denton, Texas, USA

Contributors

P. RAMACHANDRA NAIDU

Sri Venkateswara University
Tirupata, India

JAMES W. McCARGAR, SHERYL A. TUCKER, ANITA I. ZVAIGZNE

University of North Texas
Denton, Texas, USA

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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 $t/°C$, $t/°F$ or T/K as in the original; if necessary, conversions to T/K are made, sometimes in the compilations and always in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations (3) as far as possible.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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, $x_{v,1}$:

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

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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R. Cohen-Adad
Villeurbanne, France

J.W. Lorimer
London, Ont., Canada

M. Salomon
Sea Bright, NJ, USA

M.-T. Saugier-Cohen Adad
Villeurbanne, France

January, 1994

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

	x_i	w_i	m_i	c_i
$x_i =$	x_i	$\dfrac{1}{1+\dfrac{M_i}{M_c}\left(\dfrac{1}{w_i}-1+\sum\limits_{j\neq i}^{c-1}\left(\dfrac{M_c}{M_j}-1\right)\dfrac{w_j}{w_i}\right)}$	$\dfrac{1}{1+\dfrac{1}{m_i M_c}+\sum\limits_{j\neq i}^{c-1}\dfrac{m_j}{m_i}}$	$\dfrac{1}{1+\dfrac{1}{M_c}\left(\dfrac{\rho}{c_i}-M_i\right)+\sum\limits_{j\neq i}^{c-1}\dfrac{c_j}{c_i}\left(1-\dfrac{M_j}{M_c}\right)}$
$w_i =$	$\dfrac{1}{1+\dfrac{M_c}{M_i}\left(\dfrac{1}{x_i}-1+\sum\limits_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right)}$	w_i	$\dfrac{1}{1+\dfrac{1}{m_i M_i}\left(1+\sum\limits_{j\neq i}^{c-1} m_j M_j\right)}$	$\dfrac{c_i M_i}{\rho}$
$m_i =$	$\dfrac{1}{M_c\left(\dfrac{1}{x_i}-1-\sum\limits_{j\neq i}^{c-1}\dfrac{x_j}{x_i}\right)}$	$\dfrac{1}{M_i\left(\dfrac{1}{w_i}-1-\sum\limits_{j\neq i}^{c-1}\dfrac{w_j}{w_i}\right)}$	m_i	$\dfrac{1}{\dfrac{1}{c_i}\left(\rho-\sum\limits_{j\neq i}^{c-1} c_j M_j\right)-M_i}$
$c_i =$	$\dfrac{\rho}{M_i+M_c\left(\dfrac{1}{x_i}-1+\sum\limits_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right)}$	$\dfrac{\rho w_i}{M_i}$	$\dfrac{\rho}{\dfrac{1}{m_i}\left(1+\sum\limits_{j\neq i}^{c-1} M_j m_j\right)+M_i}$	c_i

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

PREFACE TO THE VOLUME

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 aforementioned ideas in mind, we have compiled published solubility data for anthracene, naphthalene, phenanthrene, pyrene, fluorene, fluoranthene, carbazole, thianthrene, and other two- and three-ring polycyclic aromatic heteroatom compounds in binary organic solvent mixtures so that experimental values will be readily available in a single reference source. Experimental data for well over 250 different systems were retrieved from the chemical literature and are compiled in this volume. Each system contains solubility data for the solute dissolved in each pure solvent and in four to ten binary solvent mixtures covering the entire range of mole fraction compositions. Literature sources searched include a complete coverage of *Chemical Abstracts* from 1907 to October 1991; Beilstein, *Handbuch der Organischen Chemie*; and the *International Critical Tables*. Polycyclic aromatic compounds are an important chemical class. They have been used as model compounds in coal liquefication process design calculations, serve as the "parent" compound or base found in a number of drug molecules, and several are common organic pollutants resulting from oil spills.

Compilations of published solubility data for crystalline polycyclic aromatic compounds dissolved 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, we have decided to include in this volume a very brief survey of select methods currently being used to estimate solute solubilities in mixed solvents. 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 editors 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

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

(3) mole fraction

$$x_i = n_i/(n_1 + n_2 + n_3 + \ldots .)\qquad [2]$$

or (4) volume fraction

$$\phi_i = n_iV_i/(n_1V_1 + n_2V_2 + n_3V_3 + \ldots .)\qquad [3]$$

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)

$$\phi_i = n_iV_{m,i}/(n_1V_{m,1} + n_2V_{m,2} + n_3V_{m,3} + \ldots .)\qquad [4]$$

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

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

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 pertubation 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).

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 preceeding 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

$$G = RT\, [\, x_1 \ln \phi_1 + x_2 \ln \phi_2 \,] \qquad [10]$$

$$\ln a_1 = \ln \phi_1 + \phi_2 (1 - V_{m,1}/V_{m,2}) \qquad [11]$$

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

$$\ln \phi_1 + (1 - \phi_1)(1 - V_{m,1}/V_{m,2}) = - \Delta H^{fus} (T_{TP} - T)/RT\, T_{TP} + \Delta C_p (T_{TP} - T)/RT$$
$$- (\Delta C_p/R) \ln (T_{TP}/T) \qquad [12]$$

Chiou and Manes (9) 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 [12]. 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. [12] (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 (10), 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 (6,11) provides reasonable estimates of solute solubility in systems containing only nonspecific interactions

$$RT \ln (a_1(s)/x_1) = V_{m,1} (1 - \phi_1)^2 (\delta_1 - \delta_{solvent})^2 \qquad [13]$$

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 (12) and Barton (11)), 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 I and II compare the predictions of eqn. [13] 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, $V_{m,\mathrm{biphenyl}}$ = 149.4 $\mathrm{cm}^3\ \mathrm{mol}^{-1}$ and $V_{m,\mathrm{naphthalene}}$ = 123.0 $\mathrm{cm}^3\ \mathrm{mol}^{-1}$, and best estimates for the solubility parameters, $\delta_{\mathrm{biphenyl}}$ = 20.05 $J^{1/2}\ \mathrm{cm}^{-3/2}$ and $\delta_{\mathrm{naphthalene}}$ = 19.84 $J^{1/2}\ \mathrm{cm}^{-3/2}$. Inspection of Tables I and II 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 $\delta_{\mathrm{solvent}}$

$$\delta_{\mathrm{solvent}} = (\phi_2\ \delta_2 + \phi_3\ \delta_3)/(\phi_2 + \phi_3) = \phi_2^{(s)}\ \delta_2 + \phi_3^{(s)}\ \delta_3 \qquad [14]$$

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. [14] into eqn. [13]

$$(1 - \phi_1)^{-2}\ RT\ \ln\ (a_1(s)/x_1) = V_{m,1}\ (\phi_2^{(s)}\ \delta_2 + \phi_3^{(s)}\ \delta_3 - \delta_1)^2 \qquad [15]$$

and multiply out the squared term

$$(1 - \phi_1)^{-2}\ RT\ \ln\ (a_1(s)/x_1) = V_{m,1}\ [\ \phi_2^{(s)}\ (\delta_2 - \delta_1)^2 + \phi_3^{(s)}\ (\delta_3 - \delta_1)^2 - \phi_2^{(s)}\ \phi_3^{(s)}\ (\delta_2 - \delta_3)^2] \qquad [16]$$

Inspection of eqn. [16] 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

$$(G_1^E)_i^\infty = (1 - \phi_1)^{-2}\ RT\ \ln\ (a_1(s)/x_1) = V_{m,1}\ (\delta_i - \delta_1)^2 \qquad i = 2,3 \qquad [17]$$

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

$$G_{23}^E = (x_2^{(s)}\ V_{m,2} + x_3^{(s)}\ V_{m,3})\ \phi_2^{(s)}\ \phi_3^{(s)}\ (\delta_2 - \delta_3)^2 \qquad [18]$$

in terms of solubility parameters.

Combining eqns. [16]-[18] one finds that the solubility of a solute in binary solvent mixtures containing only nonspecific interactions is

$$RT\ \ln\ (a_1(s)/x_1) = (1 - \phi_1)^2\ [\phi_2^{(s)}\ (G_1^E)_2^\infty + \phi_3^{(s)}\ (G_1^E)_3^\infty - V_{m,1}\ (x_2^{(s)}\ V_{m,2} + x_3^{(s)}\ V_{m,3})^{-1}\ G_{23}^E\ ] \qquad [19]$$

a volume fraction average of the solute's properties in the two pure solvents, $(G_1^E)_2^\infty$ and $(G_1^E)_3^\infty$, and a contribution due to the non-mixing of the solvent pair by the

TABLE I. 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

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

[b] Experimental solubilites were determined by Chang (54).

TABLE II. 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

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

[b] Experimental solubilities were determined by Chang (54).

presence of the solute.. Enhancement of the non-mixing term by a large solute molecule can lead to predictions of maximum ($G_{23}^E > 0$) or minimum ($G_{23}^E < 0$) mole fraction solubilities. The predictions of eqn. [19] will be compared later (in Table III) to experimental solubilities of naphthalene, 1,4-dibromobenzene, iodine, stannic iodide, 1,2-diphenyl-ethanedione, 1,4-benzoquinone, anthracene, biphenyl, pyrene and thianthrene in simple binary solvent mixtures.

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

$$- \log x_1 = - \log a_1(s) + (V_{m,1}\ \phi^2_{solvent}/2.303\ RT)\ [\delta^2_{solvent} + \delta_1^2 - 2\ \Sigma\ A_i\ \delta^i_{solvent}\ ] \qquad [20]$$

derived by Martin and co-workers (13-15) 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. [20], do enable the calculation of interpolated solubilities between two measured values and facilitate computerized storage and retrieval of experimental data. Ochsner *et al.* (16) discussed the mathematical representation of solubility data using expressions based upon mixture response-surface methods, and Acree *et al.* (17,18) 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.

THE NEARLY IDEAL BINARY SOLVENT (NIBS) MODEL

The NIBS approach was developed by Bertrand and co-workers (19-24) for describing the thermodynamic properties of a solute in binary solvent systems, and has been successful in predicting enthalpies of solution and solubilities in mixed solvents in which only nonspecific interactions are importance. The basic principles of this method as they pertain to the chemical potential of a solute will be reviewed to identify the assumptions made in the derivation of the final predictive expressions.

In the NIBS approach, expressions for the partial molar excess properties of the solute near infinite dilution were developed for a model ternary system obeying a general mixing equation

$$Z^E = (n_1\ \Gamma_1 + n_2\ \Gamma_2 + n_3\ \Gamma_3)^{-1}\ [n_1\ \Gamma_1\ n_2\ \Gamma_2\ A_{12} + n_1\ \Gamma_1\ n_3\ \Gamma_3\ A_{13} + n_2\ \Gamma_2\ n_3\ \Gamma_3\ A_{23}\ ] \qquad [21]$$

in which Z represents any extensive thermodynamic property, Γ_i is the weighting factor for component $\underline{i}$, and A_{ij} is a binary interaction parameter that is independent of composition. Through differentiation of Eqn. [21] the corresponding partial molar excess properties of the solute can be expressed in terms of a weighted mole fraction average of the infinite dilution properties in the two pure solvents, $(Z_1^E)_2^\infty$ and $(Z_1^E)_3^\infty$, and a contribution resulting from the unmixing of the binary solvent pair

$$(Z_1^E)^\infty = f_2^{(s)}\ (Z_1^E)_2^\infty + f_3^{(s)}\ (Z_1^E)_3^\infty - \Gamma_1\ (x_2^{(s)}\ \Gamma_2 + x_3^{(s)}\ \Gamma_3)^{-1}\ Z_{23}^E \qquad [22]$$

where $f_2^{(s)} = 1 - f_3^{(s)} = n_2 \Gamma_2/(n_2 \Gamma_2 + n_3 \Gamma_3)$ and $x_2^{(s)} = 1 - x_3^{(s)} = n_2/(n_2 + n_3)$.

In eqn. [22] and subsequent expressions, the superscript (∞) indicates an extrapolated value for the infinite dilution solution ($f_1 = 0$). Most of the specific elements of the model eqn. [21] were removed; only the weighting factors remain. If reasonable estimates for the weighting factors can be developed, then the thermodynamic excess properties of the solute in binary solvent systems can be predicted and compared to measured experimental data.

Weighting factors represent a measure of the skew of the binary thermodynamic excess property from mole fraction symmetry, and can be evaluated only in a relative sense, as the ratio of two weighting factors (Γ_i/Γ_j). Several methods (19-21) have been proposed previously for the evaluation of these weighting factors from the thermodynamic properties of binary mixtures. Many of these methods are not applicable in the case of solute solubility, as only a single data point is associated with each solute-solvent pair. To circumvent this problem, several simple approximations can be made: (a) approximating the weighting factors for each component by its molar volume; (b) equating the weighting factors of all components; or (c) approximating the weighting factors for each component by the surface area of the molecule.

Thermodynamic excess properties are relatively simple for directly observed excess properties such as volume and enthalpy. But in the case of Gibbs energy, thermodynamic excess properties are complicated by the fact that the total free energy of mixing is experimentally determined. The excess value must be calculated as the difference between the observed value and the value of an ideal mixture

$$G = RT \sum n_i \ln x_i + G^E \qquad [23]$$

For mixtures containing molecules with considerable differences in molar volumes, general mixing equations possessing the form of eqn. [21] more accurately describe differences between the total free energy of mixing and that predicted via the Flory-Huggins model

$$G^{mix} = RT \sum n_i \ln \phi_i + G^{FH} \qquad [24]$$

For a binary mixture, the difference between the excess Gibbs energy and the Flory-Huggins excess Gibbs energy is

$$G_{23}^{FH} = G_{23}^E + RT [\ln (x_2 V_{m,2} + x_3 V_{m,3}) - x_2 \ln V_{m,2} - x_3 \ln V_{m,3}] \qquad [25]$$

The mathematical treatment of these general mixing equations leads to two general expressions for estimating excess chemical potential of a solute at low mole fractions in a binary solvent:

$$G_1^E = (1 - f_1)^2 [f_2^{(s)} (G_1^E)_2^\infty + f_3^{(s)} (G_1^E)_3^\infty - \Gamma_1 (x_2^{(s)} \Gamma_2 + x_3^{(s)} \Gamma_3)^{-1} G_{23}^E] \qquad [26]$$

and

$$G_1^{FH} = (1 - f_1)^2 [f_2^{(s)} (G_1^{FH})_2^\infty + f_3^{(s)} (G_1^{FH})_3^\infty - \Gamma_1 (x_2^{(s)} \Gamma_2 + x_3^{(s)} \Gamma_3)^{-1} G_{23}^{FH}] \qquad [27]$$

The term G_1^{FH} represents an excess molar Gibbs energy of the solute relative to an ideal mixing equation based upon volume fractions rather than mole fractions.

Through basic thermodynamic relationships the excess chemical potential of the solute in binary solvent mixtures can be related to the solubility

$$G_1^E = RT \ln (a_1(s)/x_1) \qquad [28]$$

$$G_1^{FH} = RT \{ \ln (a_1(s)/\phi_1) - [1 - (V_{m,1}/V_{solvent})]\} \qquad [29]$$

in which $V_{m,1}$ is the molar volume of the solute in the liquid state at the desired temperature, and $a_1(s)$ is the activity of the solute referred to the hypothetical supercooled liquid below the normal melting point temperature.

Based upon different weighting factor approximations and definitions of mixture ideality, Acree and Bertrand (22-24) derived the following three NIBS expressions

$$RT \ln (a_1(s)/x_1) = (1 - x_1)^2 [x_2^{(s)} (G_1^E)_2^\infty + x_3^{(s)} (G_1^E)_3^\infty - G_{23}^E] \qquad [XX]$$

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

and

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

for predicting solubilities in binary solvents. Readers should note that the NIBS equations are named using alphabetical letters rather than numbers to permit easy identification. The first letter in the NIBS equation name indicates whether mole fractions (X) or volume fractions (V) appear inside the logarithm term, while the second letter denotes the weighting factor approximation employed, *i.e.*, V is used if $\Gamma_i = V_{m,i}$ and X is used for $\Gamma_i = \Gamma_j$, *etc*. Two additional predictive expressions involving molecular surface areas, eqns. [XA] and [VA], will be presented shortly.

As was shown in the preceeding section, eqn. [XV] can be derived from the Scatchard-Hildebrand solubility parameter theory by eliminating the three δs with the experimental solubilities in the pure solvents and the themrodynamic excess properties of the binary solvent. The NIBS treatment is more general, however, and does not place any restrictions on the numerical values that the binary interaction parameters can assume.

To illustrate the predictive application of eqn. [XX], assume that one wished to estimate the solubility of naphthalene in binary tetrachloromethane (2) + n-hexane (3) mixtures, at $x_2^{(s)} = 0.5971$ and 298.15 K, from measured solubilities in the pure solvents, $(x_1)_2 = 0.2591$ and $(x_1)_3 = 0.1168$. Begin by calculating $(G_1^E)_2^\infty$ and $(G_1^E)_3^\infty$ using $a_1(s) = 0.312$

$$(G_1^E)_2^\infty = (8.314)(298.15)\ (1 - 0.2951)^{-2} \ln (0.312/0.2591) = 838.93 \text{ J mol}^{-1}$$

$$(G_1^E)_3^\infty = (8.314)(298.15)\ (1 - 0.1168)^{-2} \ln (0.312/0.1168) = 3122.17 \text{ J mol}^{-1}$$

These values are then combined with the experimental excess Gibbs energy of the binary solvent, $G_{23}^E = 141.8 \text{ J mol}^{-1}$, to yield

$$(8.314)(298.15) \ln (0.312/x_1) = (1 - x_1)^2 [(0.5971)(838.93) + (0.4029)(3122.17) - 141.8]$$

The above expression can be solved reiteratively. Letting $(1 - x_1)^2 = 1$, generate a first approximation of $x_1 = 0.1625$, which is then used to calculate $(1 - x_1)^2$ for a second approximation. Convergence to a constant value of x_1 generally takes three or four iterations, depending upon the saturation solubility.

The predictive abilities of eqns. [XX], [XV] and [VV] are summarized in Table III for 128 systems for which solubility data and thermodynamic mixing data of the binary solvents were available at or near the same temperature. In a few instances, the Scatchard-Hildebrand solubility parameter model was used to estimate the G_{23}^{E} values required as part of the NIBS input parameters. The actual experimental solubilities of the various polycyclic aromatic compounds are tabulated in data compilation portion of this volume, which immediately follows the survey of predictive methods. Each system contains solubility data for four to ten binary solvent compositions, in addition to the measured solubilities in both pure solvents. With the exception of anthracene and pyrene solubilities in benzene + n-heptane, multiple entries for a given solute-binary solvent system indicate that more than one data set was retrieved from the chemical literature. Molar volumes and molecular surface areas used in these computations are listed in Table IV.

For the most part, eqns. [XV] and [VV] provide reasonable estimates (± 5 %) for the experimental solubilities; the exceptions being the anthracene and pyrene solubilities in solvent mixtures containing either benzene, methylbenzene or 1,4-dimethylbenzene. (These systems will be discussed in more detail later.) No attempt has been made to critically evaluate the published solubility data as only one set of measurements could be found for each system. An assessment of each data set's reliability can be gained by comparing the experimental solubilities against the various predicted values. Very close agreement between observed and predicted values suggests that each data set is internally consistent, which is further supported by the fact that plots of log x_1 versus $x_2^{(s)}$ appear as smooth curves with no noticeable outliers.

The success of eqns. [XV] and [VV] become more remarkable if one realizes that 1,2-diphenylethanedione and 1,4-benzoquinone dissolved in binary alkane + tetrachloromethane solvent mixtures cover up to a 14-fold and 6-fold range in mole fraction solubilities, respectively, despite which the observed values differ only slightly from predicted values based upon eqns. [XV] and [VV]. Stoichiometric complexation models that attribute all solubility enhancement to the formation of molecular solute-solvent complexes require at least 2 (and sometimes 3) equilibrium constants to describe these latter two sets of systems. Significant solubility enhancement can result in systems containing only nonspecific interactions. One should not naively expect that differences in nonspecific interactions, shown to be present in mixtures of two noncomplexing solvent components, to suddenly vanish whenever one of the inert solvents is replaced by a complexing solvent.

The superiority of expressions based upon molar volumes suggests that the relative sizes of the molecules are an important consideration. The use of surface areas as weighting factors may be revealing because surface area represents a different measure of molecular size. Introduction of molecular surface areas (A_i) into the basic NIBS model leads to the development of two more predictive expressions (25)

$$RT \ln (a_1(s)/x_1) = (1 - \theta_1)^2 [\theta_2^{(s)} (G_1^E)_2^{\infty} + \theta_3^{(s)} (G_1^E)_3^{\infty} - A_1 (x_2^{(s)} A_2 + x_3^{(s)} A_3)^{-1} G_{23}^E] \qquad [XA]$$

TABLE III. Comparison Between Experimental Solubilities and Predicted Values Based Upon the NIBS Equations for Nonelectrolyte Solutes Dissolved in Binary Solvent Mixtures

	RMS Deviations (%) of Calcd. Values[a]		
Binary Solvent System	[XX]	[XV]	[VV]
Solute = Naphthalene			
Benzene + cyclohexane	- 1.4	+ 1.2	- 1.1
Benzene + tetrachloromethane	+ 1.5	+ 1.7	+ 1.9
Benzene + n-hexane	+ 2.3	1.4	1.4
Cyclohexane + n-hexadecane	- 4.0	+ 2.9	+ 1.4
n-Hexane + n-hexadecane	- 6.8	+ 1.8	+ 0.8
Tetrachloromethane + cyclohexane	0.3	- 0.5	- 0.6
Tetrachloromethane + n-hexadecane	+ 8.0	+ 4.5	+ 2.4
Benzene + n-hexadecane	+ 9.2	+ 2.4	+ 0.7
Tetrachloromethane + n-hexane	+ 3.2	1.3	0.5
Cyclohexane + n-hexane	0.8	0.6	0.6
Benzene + methylbenzene	+ 0.5	0.5	+ 0.6
Tetrachloromethane + methylbenzene	- 1.5	- 1.5	- 1.5
Cyclohexane + methylbenzene	- 1.8	- 0.9	- 0.8
Ethylbenzene + tetrachloromethane	0.5	0.7	0.6
Ethylbenzene + cyclohexane	- 0.7	0.3	0.3
Solute = 1,4-Dibromobenzene			
Tetrachloromethane + n-hexadecane	+ 5.4	+ 1.8	- 0.8
n-Hexane + n-hexadecane	- 8.5	+ 1.6	0.6
Tetrachloromethane + cyclohexane	- 0.6	- 1.5	- 1.5
Solute = Stannic Iodide			
Benzene + cyclohexane	2.2	2.8	3.1
Cyclohexane + tetrachloromethane	- 0.8	- 1.3	- 1.2
Solute = Iodine			
Cyclohexane + n-hexane	+ 1.7	- 1.5	- 2.5
Cyclohexane + n-hexane	1.2	- 2.0	- 3.0
Cyclohexane + n-hexane	+ 1.6	- 1.9	- 2.0
Tetrachloromethane + n-hexane	+ 5.0	- 1.3	- 2.0
Tetrachloromethane + n-hexane	+ 5.8	- 0.8	- 1.3
Cyclohexane + n-heptane	+ 2.1	- 0.5	- 0.8
n-Heptane + n-hexadecane	- 8.2	2.4	- 1.0
2,2,4-Trimethylpentane + hexadecane	- 8.1	+ 1.8	- 0.9
Cyclohexane + tetrachloromethane	+ 0.9	- 0.7	- 0.7
Cyclohexane + OMCTS	+ 5.3	+ 4.2	- 3.0
Tetrachloromethane + OMCTS	+ 8.6	+ 5.3	- 4.5
n-Heptane + tetrachloromethane	+ 5.4	- 0.6	- 1.3
Solute = 1,2-Diphenylethanedione			
n-Hexane + cyclohexane	- 0.4	- 1.3	- 1.2
n-Hexane + tetrachloromethane	+13.0	- 3.4	- 3.1
n-Heptane + tetrachloromethane	+17.2	- 3.1	- 2.5
n-Hexane + n-heptane	- 0.6	0.3	0.3
Cyclohexane + tetrachloromethane	+ 1.5	- 2.2	- 2.4
Benzene + methylbenzene	0.2	- 0.3	- 0.3
2,2,4-Trimethylpentane + cyclohexane	+ 2.4	- 1.8	- 1.2
Cyclohexane + cyclooctane	- 2.2	0.3	0.4
n-Octane + tetrachloromethane	+25.9	- 1.8	0.9
Cyclohexane + n-octane	+ 1.8	0.6	0.3
Cyclohexane + n-heptane	+ 2.0	0.5	+ 0.7
2,2,4-Trimethylpentane + tetrachloromethane	+25.7	- 4.2	- 3.4

TABLE III. (Continued)

Solute = 1,4-Benzoquinone			
n-Octane + tetrachloromethane	+15.7	- 3.1	- 4.2
n-Heptane + tetrachloromethane	+12.4	- 3.8	- 4.4
n-Heptane + n-dodecane	- 1.4	+ 1.3	0.2
Cyclohexane + 2,2,4-trimethylpentane	0.3	0.6	- 1.1
Cyclohexane + cyclooctane	- 0.5	0.5	0.4
Cyclohexane + n-heptane	+ 0.4	- 0.5	- 0.8
Solute = Anthracene			
Cyclohexane + n-heptane	1.0	0.6	0.6
Cyclohexane + cyclooctane	- 1.4	0.9	0.9
Cyclohexane + n-octane	- 1.3	+ 0.6	+ 0.7
Cyclohexane + 2,2,4-trimethylpentane	+ 1.9	- 1.2	- 1.0
Cyclohexane + n-hexane	- 1.2	- 1.2	- 1.1
Benzene + n-heptane	+10.6	2.1	1.6
Benzene + n-heptane	+ 7.9	- 4.6	- 3.8
Benzene + cyclohexane	- 6.9	- 7.7	- 7.5
Benzene + cyclohexane	- 6.2	- 6.8	- 6.6
Benzene + tetrachloromethane	- 3.1	- 2.1	- 2.0
Benzene + n-hexane	+ 2.7	- 6.0	- 5.4
Benzene + cyclooctane	1.8	- 8.3	- 7.7
Benzene + 2,2,4-trimethylpentane	+10.5	-11.6	-10.7
Benzene + n-octane	+12.7	2.2	1.4
Benzene + methylcyclohexane	+ 2.7	- 4.7	- 4.2
Methylbenzene + n-hexane	- 1.1	- 5.7	- 5.6
Methylbenzene + cyclohexane	-12.7	-13.6	-13.4
Methylbenzene + n-heptane	+ 4.6	- 4.3	- 4.0
Methylbenzene + methylcyclohexane	- 7.4	-10.9	-10.7
Methylbenzene + n-octane	+ 8.0	- 3.6	- 3.3
Methylbenzene + 2,2,4-trimethylpentane	+14.6	1.7	1.6
Methylbenzene + cyclooctane	- 2.5	- 5.8	- 5.6
1,4-Dimethylbenzene + n-hexane	- 7.9	- 8.2	- 8.2
1,4-Dimethylbenzene + cyclohexane	-12.7	- 5.3	- 5.3
1,4-Dimethylbenzene + methylcyclohexane	-10.0	- 9.9	- 9.9
1,4-Dimethylbenzene + n-octane	+ 2.0	- 5.9	- 5.9
1,4-Dimethylbenzene + n-heptane	+ 0.7	- 4.0	- 3.9
1,4-Dimethylbenzene + 2,2,4-trimethylpentane	+10.6	0.6	0.6
Tetrachloromethane + n-hexane	+ 7.0	0.9	1.2
Tetrachloromethane + cyclohexane	0.2	- 1.5	- 1.4
Tetrachloromethane + n-heptane	+10.5	+ 2.4	+ 2.8
Tetrachloromethane + methylcyclohexane	+ 4.3	- 1.1	0.9
Tetrachloromethane + n-octane	+11.2	+ 2.3	+ 2.9
Tetrachloromethane + 2,2,4-trimethylpentane	+12.4	- 2.2	- 1.8
1,1-Oxybisbutane + n-hexane	- 5.9	0.3	0.3
1,1-Oxybisbutane + n-heptane	- 4.3	- 1.8	- 1.8
1,1-Oxybisbutane + cyclohexane	- 9.4	- 1.3	- 1.0
1,1-Oxybisbutane + methylcyclohexane	- 6.9	- 2.1	- 2.1
1,1-Oxybisbutane + n-octane	- 2.6	- 2.1	- 2.1
1,1-Oxybisbutane + 2,2,4-trimethylpentane	- 2.6	- 2.5	- 2.5
1,1-Oxybisbutane + cyclooctane	- 6.9	- 4.6	- 4.6
Solute = Biphenyl			
Cyclohexane + n-hexane	+ 1.5	+ 0.5	+ 0.5
Cyclohexane + n-octane	+ 2.7	0.6	0.6
Tetrachloromethane + n-hexane	+ 2.8	0.7	0.7
Tetrachloromethane + n-heptane	+ 4.8	0.6	+ 0.6

TABLE III. (Continued)

Cyclohexane + tetrachloromethane	0.7	+ 0.7	+ 0.7
Cyclohexane + n-heptane	+ 2.2	0.4	0.6
Solute = Pyrene			
Cyclohexane + n-hexane	- 2.9	- 2.5	- 2.4
Cyclohexane + n-heptane	- 2.3	- 1.4	- 1.0
Cyclohexane + n-octane	- 3.8	- 1.2	0.7
Cyclohexane + 2,2,4-trimethylpentane	+ 2.0	- 1.6	- 1.1
Cyclohexane + cyclooctane	- 4.3	- 1.1	- 0.9
Benzene + n-hexane	1.1	- 8.0	- 7.5
Benzene + cyclohexane	-10.0	- 9.2	- 9.1
Benzene + n-heptane	+ 5.9	- 5.6	- 4.5
Benzene + n-heptane	+ 3.6	- 9.3	- 8.4
Benzene + n-octane	+ 5.7	- 9.7	- 8.6
Benzene + cyclooctane	- 7.2	-12.0	-11.3
Benzene + 2,2,4-trimethylpentane	+10.3	-13.4	-12.2
Methylcyclohexane + 1,1-oxybisbutane	- 8.7	- 3.5	- 3.4
n-Octane + 1,1-oxybisbutane	0.8	0.8	0.8
n-Heptane + 1,1-oxybisbutane	- 6.6	- 3.5	- 3.5
Cyclohexane + 1,1-oxybisbutane	-13.4	- 3.0	- 2.5
t-Butylcyclohexane + 1,1-oxybisbutane	- 7.3	- 7.6	- 7.6
2,2,4-Trimethylpentane + 1,1-oxybisbutane	- 2.7	- 2.0	- 2.0
n-Hexane + 1,1-oxybisbutane	-10.3	- 3.0	- 2.9
Solute = Thianthrene			
Cyclohexane + n-hexane	0.3	- 1.6	- 1.3
Cyclohexane + methylcyclohexane	0.4	0.5	0.7
Cyclohexane + n-heptane	0.6	- 2.8	- 2.5
Cyclohexane + n-octane	+ 2.2	- 0.9	- 0.6
Cyclohexane + cyclooctane	- 4.9	- 1.5	- 1.3
Cyclohexane + 2,2,4-trimethylpentane	+ 4.0	- 2.5	- 2.1
Solute = Carbazole			
Cyclohexane + n-hexane	0.5	- 0.7	- 0.7
Cyclohexane + n-heptane	0.5	0.5	0.4
Cyclohexane + n-octane	- 0.8	0.6	0.8
Cyclohexane + methylcyclohexane	0.2	0.2	0.3
Cyclohexane + 2,2,4-trimethylpentane	+ 1.6	- 1.4	- 1.2
Cyclohexane + cyclooctane	- 2.7	0.5	0.5

---

[a] % RMS Deviations = $100 \{ \Sigma [\ln x_1(\text{calc})/x_1(\text{exp})]^2/N\}^{1/2}$; the algebraic sign indicates that all deviations were of the same sign.

[b] Experimental solubilities and literature references for the binary solvent properties are given elsewhere (1,20,22,23,41-53).

[c] OMCTS is used as the abbreviation of octamethylcyclotetrasiloxane.

TABLE IV. Solute and Solvent Properties used in the NIBS Predictions

Component (i)	$V_{m,i}/(\mathrm{cm}^3\ \mathrm{mol}^{-1})$	$A_i/(\mathrm{Å}^2\ \mathrm{mol}^{-1})$	$\delta_i/(\mathrm{J}^{1/2}\ \mathrm{cm}^{-3/2})^a$
Solvents			
n-Hexane	131.51	142.1	14.87
n-Heptane	147.48	160.3	15.34
n-Octane	163.46	178.4	15.42
Cyclohexane	108.76	120.8	16.75
Methylcyclohexane	128.32	137.7	16.02
2,2,4-Trimethylpentane	106.09	163.1	14.03
Cyclooctane	134.88	148.8	17.41
Benzene	89.41	109.5	18.74
Methylbenzene	106.84	126.5	18.27
1,4-Dimethylbenzene	123.93	150.3	18.06
1,1-Oxybisbutane	170.41		15.87
Tetrachloromethane	97.08		17.49
Squalane[b]	525.30		16.16
n-Hexadecane	294.12	323.2	16.34
t-Butylcyclohexane	173.93		16.00
1-Chlorobutane	105.10		17.12
1,4-Dichlorobutane	112.12		19.78
Ethylbenzene	123.06	144.9	
OMCTS[c]	314.00		
Butyl ethanoate	132.61		17.78
Diethyl hexadedioate	202.25		18.16
Solutes			
Anthracene	150.0	202.2	$(a_1(s) = 0.01049)$
Carbazole	150.0		$(a_1(s) = 0.009354)$
Thianthrene	156.0		$(a_1(s) = 0.04411)$
Naphthalene	123.0	155.8	$(a_1(s) = 0.312)$
Biphenyl	149.4	182.0	$(a_1(s) = 0.4025)$
Iodine	59.6		$(a_1(s) = 0.258)$
1,2-Diphenylethanedione	183.0		$(a_1(s) = 0.224)$
1,4-Benzoquinone	82.1		$(a_1(s) = 0.182)$
1,4-Dibromobenzene	118.0	156.6	$(a_1(s) = 0.248)$
Pyrene	166.5	213.0	$(a_1(s) = 0.1282)$
Stannic iodide	151.0		$(a_1(s) = 0.1127)$

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[a] equivalent to $\delta_i/(10^3\ \mathrm{g/kg}^{1/2}\ \mathrm{m}^{-1/2}\ \mathrm{s}^{-1})$.

[b] Squalane is 2,6,10,15,19,23-hexamethyltetracosane.

[c] OMCTS is octamethylcyclotetrasiloxane.

and

$$RT\ \{\ln\ (a_1(s)/\phi_1) - (1 - \phi_1)[1 - V_{m,1}/(x_2^{(s)}\ V_{m,2} + x_3^{(s)}\ V_{m,3})]\ \} = (1 - \Theta_1)^2\ [\Theta_2^{(s)}\ (G_1^{FH})_2^{\infty} + \Theta_3^{(s)}\ (G_1^{FH})_3^{\infty} - A_1\ (x_2^{(s)}\ A_2 + x_3^{(s)}\ A_3)^{-1}\ G_{23}^{FH}\ ] \qquad [VA]$$

depending upon whether Raoult's law (eqn. [XA]) or the Flory-Huggins model (eqn. [VA]) is used to define solution ideality.

The predictive abilities of these new equations are compared in Table V for 49 systems. The unavailability of molecular surface areas for 1,2-diphenylethanedione, 1,4-benzoquinone, tetrachloromethane, and several other solvents prevented the application of eqns. [XA] and [VA] to the remaining 79 systems considered in Table III. Equation [XA], based upon surface areas as weighting factors for the excess free energies relative to Raoult's law, is seen to be the most generally applicable predictive expression with an overall average root-mean-square (rms) deviation of about 2.0 % and a maximum error for a single data point of about 9.5 %. This maximum deviation occurs in a system (benzene + n-heptane) in which conflicting values of G_{23}^E were reported. As shown in Table V, deviations between the predicted and observed solubilities depend to a large extent upon which literature source is used for the solvent properties. This leads to two sets of predicted anthracene and pyrene solubilities that differ from each other by as much as 6 %. Discrepancies in the reported values of G_{23}^E were not noted for the remaining binary systems listed in Tables III and V. The primary advantage of eqn. [XA] over expressions based upon molar volumes, eqns. [XV] and [VV], is its applicability to anthracene and pyrene solubilities in solvent mixtures containing either benzene, methylbenzene or 1,4-dimethylbenzene. If these 29 systems are excluded from the calculations, eqns. [XV] and [VV] are slightly better than equations based upon surface areas.

Unfortunately, the present set of calculations does not clearly establish whether weighting factors are better approximated with molar volumes or surface areas. From the standpoint of calculational simplicity and the ready availability of molar volumes, eqn. [XV] is preferred, and some support for this form can be found in its adaptability to the Scatchard-Hildebrand solubility parameter theory. Similar support for eqns. [XA] and [VA] can be found in correlations of partition coefficients with surface areas and in several semi-empirical expressions developed for predicting vapor-liquid equilibrium. Equation [VV], however, is also applicable to polymer solutions, and this form of the basic NIBS model is preferred by this author because it is more ideally suited to concentration-based equilibrium constants and to gas-liquid chromatographic partition coefficients. Furthermore, Chiou and Manes (9) have shown that the Flory-Huggins model, upon which eqn. [VV] is based, represents a more realistic description of ideality in systems having molecules of moderate size disparity.

EXTENDED NIBS MODEL FOR SYSTEMS HAVING SOLUTE-SOLVENT COMPLEXATION

An early detailed treatment of association equilibria was presented by Gibbs (26). He considered the anomalous vapor densities of compounds like nitrogen dioxide and acetic acid, and concluded that these compounds must be strongly associated. By

TABLE V. Comparison Between Experimental Solubilities and Predicted Values Based Upon the NIBS Equations [XA] and [VA]

Binary Solvent System	RMS Deviations (%) of Calcd. Values[a] [XA]	[VA]
Solute = Naphthalene		
Benzene + cyclohexane	+ 0.4	+ 0.6
Benzene + n-hexane	+ 1.9	+ 2.2
Cyclohexane + n-hexadecane	+ 2.8	+ 1.5
n-Hexane + n-hexadecane	+ 1.7	+ 0.6
Benzene + n-hexadecane	+ 3.3	+ 2.5
Cyclohexane + n-hexane	0.8	0.8
Benzene + methylbenzene	+ 0.5	+ 0.7
Cyclohexane + methylbenzene	+ 1.0	+ 1.0
Ethylbenzene + cyclohexane	+ 1.4	+ 1.5
Solute = Anthracene		
Cyclohexane + n-heptane	0.6	+ 1.0
Cyclohexane + cyclooctane	+ 1.0	+ 1.2
Cyclohexane + n-octane	+ 0.9	+ 1.5
Cyclohexane + 2,2,4-trimethylpentane	+ 0.5	+ 1.1
Cyclohexane + n-hexane	0.3	0.3
Benzene + n-heptane	+ 5.9	+ 6.9
Benzene + n-heptane	+ 2.1	+ 3.1
Benzene + cyclohexane	- 1.8	- 1.7
Benzene + cyclohexane	1.1	1.1
Benzene + n-hexane	+ 2.6	+ 3.1
Benzene + cyclooctane	- 3.6	3.0
Benzene + 2,2,4-trimethylpentane	+ 1.8	+ 3.0
Benzene + n-octane	+ 4.0	+ 5.2
Benzene + methylcyclohexane	2.9	3.5
Methylbenzene + n-hexane	0.9	1.0
Methylbenzene + n-heptane	1.3	+ 1.6
Methylbenzene + methylcyclohexane	- 5.7	- 5.6
Methylbenzene + n-octane	1.3	+ 1.8
Methylbenzene + cyclooctane	1.1	- 1.7
1,4-Dimethylbenzene + n-hexane	- 2.0	- 2.0
1,4-Dimethylbenzene + cyclohexane	0.6	0.6
1,4-Dimethylbenzene + methylcyclohexane	- 5.1	- 5.1
1,4-Dimethylbenzene + n-octane	- 1.3	- 1.2
1,4-Dimethylbenzene + n-heptane	+ 1.2	+ 1.4
Solute = Biphenyl		
Cyclohexane + n-hexane	+ 1.4	+ 1.5
Cyclohexane + n-octane	+ 0.9	+ 1.1
Cyclohexane + n-heptane	+ 1.0	+ 1.1
Solute = Pyrene		
Cyclohexane + n-hexane	- 1.6	- 1.4
Cyclohexane + n-heptane	- 0.8	0.4
Cyclohexane + n-octane	0.8	0.4
Cyclohexane + 2,2,4-trimethylpentane	0.5	+ 1.0
Cyclohexane + cyclooctane	- 1.0	- 0.7
Benzene + n-hexane	2.0	2.1
Benzene + cyclohexane	- 4.2	- 4.2
Benzene + n-heptane	+ 2.1	+ 2.8
Benzene + n-heptane	2.8	2.3

TABLE V. (Continued)

Benzene + n-octane	- 4.0	- 2.8
Benzene + cyclooctane	- 7.6	- 7.1
Benzene + 2,2,4-trimethylpentane	0.8	+ 1.5
Solute = 1,4-Dibromobenzene		
n-Hexane + n-hexadecane	+ 1.7	0.5

---

[a] % RMS Deviation = $100 \{ \Sigma [\ln x_1(\text{calc})/x_1(\text{exp})]^2/N\}^{1/2}$; the algebraic sign indicates that all deviations were of the same sign.

[b] Experimental solubilities and literature references for the binary solvent properties are given elsewhere (1,23,44-47,50).

attributing deviations from the expected vapor densities solely to the formation of associated molecules, and by assuming that the individual monomeric and associated species obeyed the ideal gas law, Gibbs calculated equilibrium constants and formation enthalpies for reactions such as

$$2\ NO_2 \rightleftharpoons N_2O_4$$
$$2\ CH_3COOH \rightleftharpoons (CH_3COOH)_2$$
$$PCl_3 + Cl_2 \rightleftharpoons PCl_5$$

The basic idea that association parameters can be inferred by observing deviations from an idealized relation has persisted almost without modification to the present. In fact, it is fair to state that virtually all published thermodynamic constants for complexation reactions have been obtained by comparing experimental results on associating systems with expectations from some ideal law or combination of laws.

It is not difficult to identify distinct schools of thought regarding the propriety of various methods for treating experimental data to obtain association parameters. At one extreme are those who, with Dolezalek (27,28), ascribe all deviations from ideality to the formation of chemical compounds between interacting molecules. Negative deviations from Raoult's law are rationalized in terms of the assumed existence of heteromolecular complexes, while positive deviations are attributed to the formation of homomolecular complexes between molecules of the individual components. However, there have been numerous challenges to the assumption that all deviations from the ideal solution are chemical in origin. Quite early, van Laar (29-31) advocated the concept that physical factors that are too weak to stabilize discrete molecular aggregates lead to nonideality in nonelectrolyte solutions. Molecular theories of liquid mixtures, such as the Scatchard-Hildebrand solubility parameter model, can account for fairly sizeable deviations from Raoult's law in systems where chemical effects are presumably absent. Consequently, it is often argued that complex formation should be considered to occur only to the extent that solution nonideality exceeds that predicted by models based upon nonspecific physical interactions. There is, as one can imagine, still considerable ground for disagreement concerning the quantitative contributions of physical effects in associating systems, or stated differently, the degree to which activity coefficient effects complicate the interpretation of experimental data. These ambiguities clearly make it difficult to develop meaningful descriptions and explanations of solution nonideality, particularly in the case of weak association complexes.

The chemical and physical descriptions of solutions represent extreme, one-sided statements of what thermodynamicists believe to be the actual situation. Generally, both physical and chemical forces should be taken into account. A comprehensive theory of liquid solutions should provide for a smooth transition from one limit of an entirely physical description to the other limit of a completely chemical description. It is, of course, difficult to formulate theories that take into account the physical and chemical effects, as the mathematics become complex and the number of adjustable parameters rapidly increases. Nevertheless, a few classical attempts have been made and in this section the Extended NIBS approach for describing the solubility behavior of crystalline solutes in complexing systems will be discussed in detail.

The success of eqn. [VV] in predicting solubilities in binary solvent mixtures with molar volumes covering a three-fold range and for solutes encompassing up to a 14-fold range of mole fraction solubilities suggests that this expression should provide adequate estimates of the physical contributions to nonideality in systems containing chemical interactions such as those between the solute and a complexing solvent. Application of the Flory-Huggins form of the basic NIBS mixing model to the quarternary system (A_1, B, C_1, AC)

$$A_1 + C_1 \rightleftharpoons AC \qquad K_{AC}^{\phi} = \phi_{AC}/(\phi_{A1}\,\phi_{C1}) \qquad [30]$$

takes the form

$$\begin{aligned} G = {} & RT\,[\, n_{A1} \ln \phi_{A1} + n_B \ln \phi_B + n_{C1} \ln \phi_{C1} + n_{AC} \ln \phi_{AC} \,] + \\ & (n_{A1} V_{m,A1} + n_B V_{m,B} + n_{C1} V_{m,C1} + n_{AC} V_{m,AC})\,[\phi_{A1}\,\phi_B\,A_{A1B} + \phi_{A1}\,\phi_{C1}\,A_{A1C1} \\ & + \phi_{A1}\,\phi_{AC}\,A_{A1AC} + \phi_B\,\phi_{C1}\,A_{BC1} + \phi_B\,\phi_{AC}\,A_{BAC} + \phi_{C1}\,\phi_{AC}\,A_{C1AC}\,] \qquad [31] \end{aligned}$$

the only assumption being that the molar volume of the AC-complex equals the sum of the molar volumes of components A and C, that is, $V_{m,AC} = V_{m,A} + V_{m,C}$. Through suitable mathematical manipulations and simplifying approximations for the three binary interaction parameters involving the molecular complex, eqn. [31] can be transformed into the following expression

$$\begin{aligned} RT\,[\ln (a_A(s)/\phi_{A1}) - 1 + V_{m,A}/V_{soln}\,] = {} & (1 - \phi_A)^2\,[\phi_B^{(s)}\,(G_A^{FH})_B^{\infty} + \phi_C^{(s)}\,(G_A^{FH})_C^{\infty} \\ & - V_{m,A}\,(x_B^{(s)}\,V_{m,B} + x_C^{(s)}\,V_{m,C})^{-1}\,G_{BC}^{FH}\,] \qquad [32] \end{aligned}$$

for describing the solubility of a crystalline solute (component A) in binary solvent mixtures, where

$$(G_A^{FH})_B^{\infty} = RT\,(1 - \phi_A)^{-2}\,[\,\ln (a_A(s)/\phi_A) - (1 - \phi_A)(1 - V_{m,A}/V_{m,B})] \qquad [33]$$

$$(G_A^{FH})_C^{\infty} = RT\,(1 - \phi_A)^{-2}\,[\,\ln (a_A(s)/\phi_{A1}) - 1 + \phi_{A1} + \phi_C(V_{m,A}/V_{m,C})] \qquad [33]$$

$$1/V_{soln} = \phi_{A1}/V_{m,A} + \phi_B/V_{m,B} + \phi_{C1}/V_{m,C1} + \phi_{AC}/V_{m,AC} \qquad [34]$$

Calculation of the solute-solvent equilibrium using eqn. [32] is relatively straightforward. The quantities $(G_A^{FH})_B^{\infty}$ and $(G_A^{FH})_C^{\infty}$ are calculated from the measured volume fraction solubility of the solute

$$\phi_A = \phi_{A1}\,[1 + V_{m,A}\,K_{AC}^{\phi}\,\phi_{C1}/(V_{m,A} + V_{m,C})] \qquad [35]$$

in the pure solvents using an assumed value for the equilibrium constant. These quantities, along with the excess Gibbs energy of the binary solvent mixture, are then used in eqn. [32] to calculate ϕ_A via an iterative approach. One continues to vary K_{AC}^{ϕ} until one obtains a numerical value that best describes the experimental solubilities in a particular binary solvent mixture.

When the solubility is sufficiently small, $\phi_A \approx 0$ and $1 - \phi_A \approx 1$, reasonable estimates of K_{AC}^{ϕ} are often obtainable from a simplified form of eqn. [32] relating the overall solute solubility in the binary solvent mixture to the solubility in the two pure solvents, $(\phi_A)_B$ and $(\phi_A)_C$.

$$\ln(\phi_A) = \phi_B^{(s)} \ln(\phi_A)_B + \phi_C^{(s)} \ln(\phi_A)_C + \ln[1 + V_{m,A} K_{AC}^{\phi} \phi_C^{(s)}/(V_{m,A} + V_{m,C})]$$
$$- \phi_C^{(s)} \ln[1 + V_{m,A} K_{AC}^{\phi}/(V_{m,A} + V_{m,C})] - V_{m,A} (RT)^{-1} (x_B^{(s)} V_{m,B} + x_C^{(s)} V_{m,C})^{-1} G_{BC}^{FH} \qquad [37]$$

In the absence of solute-solvent complexation, $K_{AC}^{\phi} = 0$, eqns. [32] and [37] correctly reduce to eqn. [VV] of the basic NIBS model, thereby providing a smooth transition between complexing and noncomplexing systems.

To calculate the equilibrium constant, substitute the solute solubility at a particular solvent composition (*i.e.*, $\phi_B^{(s)} = 0.5$) into eqn. [37] and solve the resulting mathematical expression for K_{AC}^{ϕ}. For example, to evaluate the carbazole-bisoxybutane association constant from the carbazole solubility in the n-hexane (B) + 1,1,-oxybisbutane (C) system at $x_C^{(s)} = 0.3404$ ($\phi_C^{(s)} = 0.4007$), one would need to solve

$$\ln 0.001208 = (0.5993) \ln 0.0001585 + (0.4007) \ln 0.004414$$
$$+ \ln[1 + K_{AC}^{\phi} (150.00)(0.4007)/(324.41)]$$
$$- (0.4007) \ln[1 + K_{AC}^{\phi} (150.00)/(324.71)]$$
$$+ [(150.00)(49.04)/(8.314)(298.15)(144.75)]$$

obtaining a numerical of $K_{AC}^{\phi} = 24.0$. Volume fraction compositions of carbazole used in the preceding example were

$$(\phi_A)_C = (0.005011)(150.00)/[(0.005011)(150.00) + (0.994989)(170.41)] = 0.004414$$
$$(\phi_A)_B = (0.000139)(150.00)/[(0.000139)(150.00) + (0.999861)(131.51)] = 0.0001585$$
$$\phi_A = (0.001166)(150.00)/[(0.001166)(150.00) + (0.998834)(144.75)] = 0.001208$$

calculated from the experimental solubilities (which are listed in the compilation portion of this volume) using the ideal molar volume approximation. Excess Gibbs energy of the binary solvent mixture, $G_{BC}^{FH} = 49.04$ J mol^{-1}, was estimated from the solubility parameter model, with $\delta_{\text{hexane}} = 14.87$ J$^{1/2}$ cm$^{-3/2}$ and $\delta_{\text{oxybisbutane}} = 15.87$ J$^{1/2}$ cm$^{-3/2}$.

McCargar and Acree (32-35) showed that the Extended NIBS model can be used to calculate solute-solvent association constants from the measured solubility in binary solvent mixtures. Calculated carbazole-oxybisbutane equilibrium constants are summarized in Table VI for the ten inert hydrocarbon cosolvents the authors considered. Inspection of Table VI reveals that the Extended NIBS model does mathematically describe the experimental solubilities to within an average absolute deviation of ± 2 % using a single association constant, indicating that the solubility data is both internally consistent and that there are no obvious outliers (incorrect entries) in the ten data sets. Calculated K_{AC}^{ϕ} values do vary slightly with inert cosolvent, the numerical values ranging from $K_{AC}^{\phi} = 22$ for n-heptane solvent to an upper limit of $K_{AC}^{\phi} = 30$ for 2,2,4-trimethylpentane and t-butylcyclohexane. The success of the Extended NIBS model is even more remarkable if one realizes that the mole fraction solubilities of carbazole covered up to a 35-fold range, and that the inert hydrocarbon cosolvents included both small (cyclohexane, n-hexane) and large (n-hexadecane, squalane) alkanes. Also included in Table VI are calculated association constants for *presumed* anthracene-diethyl hexanedioate (36), anthracene-butyl ethanoate (37), anthracene-chlorobutane (38), pyrene-dichlorobutane (39) and anthracene-dichlorobutane (40) molecular

TABLE VI. Volume Fraction and Mole Fraction Based Association Constants for Presumed Solute-Solvent Molecular Complexes

Inert Hydrocarbon	$K_{AC}^{\phi,a}$	% Dev.[b]	$K_{AC}^{x,a}$	% Dev.[b]
Complex = Carbazole-Oxybisbutane				
n-Hexane	24.0	2.0	15.2	2.0
n-Heptane	22.0	1.8	12.0	1.8
n-Octane	25.0	1.7	12.5	1.6
Cyclohexane	24.0	2.2	18.5	1.8
Methylcyclohexane	26.0	1.8	17.0	1.6
Cyclooctane	25.0	2.1	15.5	2.1
2,2,4-Trimethylpentane	30.0	1.7	14.0	1.4
n-Hexadecane	24.0	1.4	6.3	1.4
Squalane[c]	23.0	1.7	3.5	1.6
t-Butylcyclohexane	30.0	1.5	14.0	1.7
Complex = Anthracene-Diethyl hexanedioate				
n-Hexane	10.5	0.6		
n-Heptane	10.5	0.9		
n-Octane	10.5	0.9		
Cyclohexane	13.0	1.6		
Methylcyclohexane	12.5	1.1		
2,2,4-Trimethylpentane	9.0	1.8		
Complex = Anthracene-Butyl ethanoate				
n-Hexane	5.5	0.3	3.0	0.5
n-Heptane	5.8	0.4	2.7	0.6
n-Octane	5.5	0.6	2.4	1.0
Cyclohexane	8.0	1.5	5.9	1.3
Methylcyclohexane	8.0	0.9	4.1	0.4
2,2,4-Trimethylpentane	4.5	1.3	1.7	0.8
Complex = Anthracene-Chlorobutane				
n-Hexane	3.5	0.6		
n-Heptane	3.5	0.6		
n-Octane	3.0	0.6		
Cyclohexane	6.0	1.3		
Methylcyclohexane	5.0	0.3		
2,2,4-Trimethylpentane	2.5	1.0		
Complex = Anthracene-Dichlorobutane				
n-Heptane	8.5	0.9		
n-Octane	8.0	1.1		
Cyclohexane	12.0	1.2		
Methylcyclohexane	10.0	1.0		
Complex = Pyrene-Dichlorobutane				
n-Hexane	13.5	1.6		
n-Heptane	15.0	1.2		
n-Octane	12.5	1.8		
Cyclohexane	18.0	1.9		
Methylcyclohexane	15.0	1.1		
2,2,4-Trimethylpentane	11.0	3.9		

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[a] Scatchard-Hildebrand solubility parameter model was used to estimate G_{BC}^{E}. Association parameters are subject to re-evaluation whenever binary solvent

TABLE VI. (Continued)

properties become available.

[b] % Dev. = $(100/N)\ \Sigma\ \left| \ln [x_1(\mathrm{cal})/x_1(\mathrm{exp})] \right|$.

[c] Squalane is 2,6,10,15,19,23-hexamethyltetracosane.

complexes. Again the Extended NIBS model described the solubility behavior to within ± 3 %, and there was no indication that any individual data point was in error.

Volume fraction-based carbazole-oxybisbutane equilibrium constants do vary slightly with inert cosolvent, and one naturally wonders if a mole fraction-based constant, K_{AC}^{x},

$$A_1 + C_1 \rightleftharpoons AC \qquad K_{AC}^{x} = x_{AC}/(x_{A1}\, x_{C1}) \qquad [38]$$

would be more appropriate. Volume fraction-based constants are consistent with the Flory-Huggins model definition of mixture ideality, whereas mole fraction concentrations are consistent with an ideal mixture defined in terms of Raoult's law. Modification of the entropic contribution eqn. [32] to include Raoult's law leads to the following expression

$$\ln x_A = \phi_B^{(s)} \ln (x_A)_B + \phi_C^{(s)} \ln (x_A)_C + \ln [1 + K_{AC}^{x}\, x_C^{(s)}] - \phi_C^{(s)} \ln [1 + K_{AC}^{x}] + V_{m,A}\, (RT)^{-1}\, (x_B^{(s)}\, V_{m,B} + x_C^{(s)}\, V_{m,C})^{-1}\, G_{BC}^{E} \qquad [39]$$

for solute solubility in a binary solvent. Again it has been assumed that the solute has a very limited solubility so that $1 - x_A = 1$ and $x_{C1} = x_C^{(s)}$. The rigorous derivation of eqn. [39] appears in the chemical literature (35).

Table VI summarizes the descriptive ability of eqn. [39] for carbazole solubilities in the ten binary alkane + 1,1-oxybisbutane solvent mixtures. Surprisingly, this particular form of the Extended NIBS model also describes the solubility data to an average deviation of about ± 2 %, despite the fact that considerable molecular size disparity exists in both the n-hexadecane + 1,1-oxybisbutane and squalane + 1,1,-oxybisbutane mixtures. The molar volume of squalane, $V_{m,\mathrm{squalane}}$ = 525.30 cm^3 mol^{-1}, is over three times greater than the molar volume of 1,1-oxybisbutane, $V_{m,\mathrm{oxybisbutane}}$ = 170.41 cm^3 mol^{-1}. Comparable descriptive abilities suggest that it may be impossible to resolve questions regarding the superiority between eqns. [37] and [39] solely on the basis of experimental solubilities in a single binary solvent system. If all ten systems are considered as a whole, however, one discovers that the volume fraction-based equilibrium constants are more independent of the inert hydrocarbon cosolvent. Numerical values of the volume fraction equilibrium constant vary by about 36 %, while the mole fraction constant of K_{AC}^{x} = 18.5 for cyclohexane is more than five times greater that K_{AC}^{x} = 3.5 for squalane cosolvent. Equations [37] and [39] theoretically require that the equilibrium parameters depend only upon pure-component chemical potentials (μ_A^*, μ_C^* and μ_{AC}^*), molar volumes of components A and C, and the A_{A1C1} binary interaction parameter which was initially used in modelling the quarternary system (A_1, B, C_1, AC).

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 the NIBS model, one started with the prior knowledge that the basic model described experimental solubilities in a large number of binary solvent mixtures containing only nonspecific interactions. The Extended NIBS model and expressions derived therefrom mathematically describe the solubility behavior of carbazole in binary alkane + 1,1-oxybisbutane, of anthracene in binary alkane + diethyl hexanedioate, of anthracene in binary alkane + butyl ethanoate, and of anthracene in binary alkane + chloroalkane 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 and that there are no obvious outliers. Models, such as the NIBS and Extended NIBS models, do provide a 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.

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

$$(Z^E_{ABC})^{exp} - (Z^E_{ABC})^{calc} = x_A \, x_B \, x_C \, Q_{ABC} \qquad [40]$$

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

$$Q_{ABC} = A_{ABC} + \Sigma \; B_{AB}^{(i)} \, (x_A - x_B)^i + \Sigma \; B_{AC}^{(j)} \, (x_A - x_C)^j + \Sigma \; B_{BC}^{(k)} \, (x_B - x_C)^k \qquad [41]$$

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 (17,18,54) suggested possible mathematical representations for isothermal solubility data based upon either a Combined NIBS/Redlich-Kister model

$$\ln x_A = x_B^{(s)} \ln (x_A)_B + x_C^{(s)} \ln (x_A)_C + x_B^{(s)} x_C^{(s)} \; \Sigma \; S_1 \, (x_B^{(s)} - x_C^{(s)})^i \qquad [42]$$

or Modified Wilson equation

$$\ln (a_A(s)/x_A) = 1 - x_B^{(s)} \{1 - \ln [a_A(s)/(x_A)_B]\}/(x_B^{(s)} + x_C^{(s)} \Lambda_{BC}^{adj})$$
$$- x_C^{(s)} \{1 - \ln [a_A(s)/(x_A)_C]\}/(x_B^{(s)} \Lambda_{CB}^{adj} + x_C^{(s)}) \qquad [43]$$

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 [43] is given in Tables VII and VIII, respectively. Careful examination of Table VII reveals that eqn. [43] provides a reasonable mathematical representation of the carbazole solubility data in all 16 systems considered, which cover up to a 40-fold and 340-fold range in mole fraction solubilities in the case of 2,2,4-trimethylpentane + 1,1-oxybisbutane and 2,2,4-trimethylpentane + tetrahydropyran. The actual experimental solubilities are given in the data compilation portion of this volume. Back-calculated and experimental values generally differ by less than ± 3 %. Surprisingly, this simple two-parameter expression is able to imitate the sharp, pronounced solubility enhancement that occurs when both 1,1-oxybisbutane and tetrahydropyran are initially added to a pure alkane cosolvent. Carbazole solubilities increase between 5- and 15-fold by the time the tetrahydropyran mole fraction reaches $x_{THP} = 0.15$.

Based upon spectroscopic studies on similar mixtures, carbazole is expected to interact with both ethers to form a 1:1 carbazole-ether association complex. Complexation with tetrahydropyran is further suggested by the fact that the measured carbazole solubility far exceeds the activity of the solid solute, *i.e.*, $x_A > a_A(s)$. The calculated activity coefficient of carbazole in pure tetrahydropyran is considerably less than unity, $\gamma_A^{sat} = a_A(s)/(x_A)_{THP} = 0.218$, indicating substantial negative deviations from Raoult's Law. Included in Table VII are similar calculations for anthracene dissolved in select binary solvent mixtures. While eqn. [43] does describe the solubility data as a whole, it should be noted that there may be one or two individual data points within each system for which deviations may exceed ± 6 %.

During the course of evaluating parameters for the Modified Wilson equation, the authors noted that on a Λ_{BC}^{adj} versus Λ_{CB}^{adj} versus % Deviation three-dimensional map there existed several parameter pairs which described the carbazole solubility to within the quoted uncertainty. For example, in the case of carbazole solubilities in 2,2,4-trimethylpentane + tetrahydropyran mixtures, the percent deviation was approximately 4 % for $\Lambda_{BC}^{adj} = 1.300$ and $\Lambda_{CB}^{adj} = 0.14$, 2.6 % for $\Lambda_{BC}^{adj} = 1.25$ and $\Lambda_{CB}^{adj} = 0.12$, and 1.8 % for $\Lambda_{BC}^{adj} = 1.188$ and $= \Lambda_{CB}^{adj} = 0.107$. No special attempt was made to optimize calculated Λ_{ij}^{adj} values as the authors wished only to learn if eqn. [43] could be used to mathematically represent experimental data in systems covering extremely large solubility ranges. Any parameter set having ± 2.5 % (quoted experimental uncertainty in the alkane + dibutyl ether systems) was sufficient for this purpose.

In comparison, the two-parameter form of eqn. [42] failed badly to describe the carbazole solubility data as the average absolute deviations were about 15-25 %. Many of these systems have highly skewed ln x_A versus $x_B^{(s)}$ curves caused by the large initial solubility enhancement, and will necessitate expanding the Redlich-Kister powere series by at least 2 (perhaps more) additional terms. Similar failures in the Redlich-Kister equation can be found in the chemical literature in the mathematical representation of exces enthalpy data for highly nonideal alcohol + hydrocarbon mixtures. Linear least squares analysis of

$$[\ln x_A - x_B^{(s)} \ln (x_A)_B + x_C^{(s)} \ln (x_A)_C]/ x_B^{(s)} x_C^{(s)} \qquad [44]$$

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

Solvent (B) + Solvent (C)	$\Lambda_{ij}^{adj,a}$	% Dev.[b]
<u>Solute = Carbazole</u>		
t-Butylcyclohexane + tetrahydropyran	1.151 0.116	1.5
n-Hexane + tetrahydropyran	2.280 0.0560	1.1
n-Hexadecane + tetrahyropyran	0.650 0.219	3.2
Cyclohexane + tetrahydropyran	1.800 0.0900	1.6
n-Heptane + tetrahydropyran	1.405 0.106	3.3
2,2,4-Trimethylpentane + tetrahydropyran	1.188 0.107	1.8
n-Hexane + 1,1-oxybisbutane	2.349 0.0100	2.6
n-Heptane + 1,1-oxybisbutane	2.179 0.0308	1.5
n-Octane + 1,1-oxybisbutane	2.188 0.0287	2.4
Methylcyclohexane + 1,1-oxybisbutane	2.897 0.0195	1.7
Cyclooctane + 1,1-oxybisbutane	3.113 0.0110	1.5
n-Hexadecane + 1,1-oxybisbutane	2.630 2.985	1.6
Squalane + 1,1-oxybisbutane	1.860 4.390	1.5
t-Butylcyclohexane + 1,1-oxybisbutane	2.520 0.0260	1.8
2,2,4-Trimethylpentane + 1,1-oxybisbutane	2.321 0.00833	2.0
Cyclohexane + 1,1-oxybisbutane	2.926 0.000	2.2
<u>Solute = Anthracene</u>		
n-Hexane + dibutyl oxalate	3.825 0.290	0.8
n-Heptane + dibutyl oxalate	3.323 0.304	0.6
n-Octane + dibutyl oxalate	3.263 0.308	0.7
Cyclohexane + dibutyl oxalate	5.353 0.279	0.3
Methylcyclohexane + dibutyl oxalate	6.037 0.345	0.5
2,2,4-Trimethylpentane + dibutyl oxalate	4.302 0.514	0.4

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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. = $(100/N)\ \Sigma\ |\ \ln\ [x_A(\mathrm{cal})/x_A(\mathrm{exp})]\ |$.

TABLE VIII. Mathematical Representation of Carbazole and 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]
Solute = Carbazole				
t-Butylcyclohexane + tetrahydropyran	5.473 4.931	17.8	4.250 2.901 4.024 3.878	2.6
n-Hexane + tetrahydropyran	8.415 6.558	19.7	6.951 5.102 5.739 4.806	1.9
n-Hexadecane + tetrahyropyran	2.971 3.216	11.6	2.103 2.001 2.776 1.992	1.3
Cyclohexane + tetrahydropyran	7.153 5.214	18.4	5.901 4.004 4.265 3.495	3.8
n-Heptane + tetrahydropyran	6.863 6.334	25.8	4.853 2.551 5.161 5.564	3.3
2,2,4-Trimethylpentane + tetrahydropyran	5.582 4.407	14.6	4.720 2.998 3.272 4.012	4.2
n-Hexane + 1,1-oxybisbutane	3.850 3.388	10.7	3.250 1.671 1.865 3.211	2.1
n-Heptane + 1,1-oxybisbutane	3.229 2.490	5.5	2.921 1.999 1.369	2.9
n-Octane + 1,1-oxybisbutane	3.209 2.190	7.1	2.650 2.001 2.204	1.7
Methylcyclohexane + 1,1-oxybisbutane	4.035 3.209	10.1	3.398 2.302 2.316 1.137	1.9
n-Hexadecane + 1,1-oxybisbutane	1.618 1.092	2.7		
Cyclooctane + 1,1-oxybisbutane	3.829 3.105	10.9	3.200 1.998 2.074 1.856	2.7
Squalane + 1,1-oxybisbutane	0.517 0.592	1.6		
t-Butylcyclohexane + 1,1-oxybisbutane	3.328 2.379	6.7	2.848 2.332 1.736	2.2

TABLE VIII. (Continued)

2,2,4-Trimethylpentane + 1,1-oxybisbutane	3.648	7.1	3.150	2.3
	2.752		1.951	
			1.964	
			1.598	
Cyclohexane + 1,1-oxybisbutane	4.286	13.7	3.615	3.7
	4.438		2.750	
			2.387	
			2.067	
<u>Solute = Anthracene</u>				
n-Hexane + dibutyl oxalate	2.716	5.0	2.350	0.7
	1.765		1.449	
			1.375	
n-Heptane + dibutyl oxalate	2.252	3.0	2.100	1.0
	1.305		1.156	
			0.626	
n-Octane + dibutyl oxalate	2.065	3.0	1.860	0.4
	1.076		0.988	
			0.712	
Cyclohexane + dibutyl oxalate	2.714	6.0	2.400	2.0
	2.256		1.726	
			1.368	
Methylcyclohexane + dibutyl oxalate	2.512	5.6	2.100	1.2
	1.929		1.567	
			1.550	
2,2,4-Trimethylpentane + dibutyl oxalate	2.512	4.1	2.250	0.9
	1.519		1.348	
			0.968	

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

versus $x_B^{(s)} - x_C^{(s)}$ leads to abnormally large S_0 and S_1 values as the two-parameter form of eqn. [42] tries to describe the solubility behavior near the pure alkane cosolvent. Unfortunately, even with these large "curve-fit" parameters, eqn. [42] still underpredicts the initial carbazole solubilities in binary n-hexane + tetrahydropyran, n-heptane + tetrahydropyran, cyclohexane + tetrahydropyran, and 2,2,4-trimethylpentane + tetrahydropyran mixtures by as much as 25 %. At mole fraction compositions near $x_B^{(s)} = 0.5$, eqn. [42] has overcompensated for the high initial skew and now the back-calculated solubilities are much too large.

Unlike the Modified Wilson model discussed above, eqn. [42] does contain provisions for additional parameterization. Examination of Table VIII further reveasl that eqn. [42] requires 3 or 4 parameters to describe 13 of the 16 carbazole systems to within an average deviation of 3.5 %. Slightly larger average deviations of 3.8 % and 4.2 % were noted in cyclohexane + tetrahydropyran and 2,2,4-trimethylpentane + tetrahydropyran mixtures where the reproducibility in measured carbazole solubilities was about $\pm$ 4 %. Again, there may be one or two individual data points within each system for which the deviation exceeds $\pm$ 6 %.

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 and carbazole solubility data. For this latter set of systems there were no other convenient means to critically evaluate the published isothermal solubility data. The simple NIBS expressions based upon only nonspecific interactions are not applicable because of strong solute-solvent complexation. Lack of excess Gibbs energy data for the fairly nonideal alkane + tetrahydropyran solvent systems prevented one from using the Extended NIBS model. Many of the systems discussed as part of the NIBS comparisons (see Tables III and V) covered less than a 10-fold mole fraction range, and they too can be described by either the Combined NIBS/Redlich-Kister (eqn. [42]) or Modified Wilson (eqn. [43]) mathematical representation. In all of the computations performed to date, we failed to find any experimental data in need of redetermination.

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ACENAPHTHENE SOLUBILITES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

None

II. Alkane + Aromatic Hydrocarbon

cyclohexane + benzene

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + pyridine
cyclohexane + pyridine
benzene + thiophene
cyclohexane + thiophene
thiophene + pyridine
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_2^{(s)}$	x_1	T/K	$x_2^{(s)}$	x_1
306.55	0.0000	0.2253	303.95	0.7000	0.1333
312.95	0.0000	0.2724	314.55	0.7000	0.2015
319.85	0.0000	0.3309	325.25	0.7000	0.3032
328.05	0.0000	0.4158	333.45	0.7000	0.4059
335.95	0.0000	0.5101	339.95	0.7000	0.5084
345.75	0.0000	0.6498			
			303.35	1.0000	0.0853
312.75	0.3000	0.2467	307.35	1.0000	0.1031
319.65	0.3000	0.3050	312.05	1.0000	0.1274
333.25	0.3000	0.4545	316.45	1.0000	0.1565
338.55	0.3000	0.5240	320.95	1.0000	0.1931
344.55	0.3000	0.6148	325.65	1.0000	0.2421
			329.95	1.0000	0.2984
314.45	0.5000	0.2400	334.65	1.0000	0.3697
325.85	0.5000	0.3459	339.85	1.0000	0.4645
333.15	0.5000	0.4347	346.45	1.0000	0.5992
343.15	0.5000	0.5815	354.45	1.0000	0.7742
350.25	0.5000	0.7010			

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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, Milwaukee, Wisconsin, USA, was used as received.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data <u>1985</u>, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data <u>1987</u>, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. <u>1983</u>, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
306.55	0.0000	0.2253	340.3	0.3000	0.5775
312.95	0.0000	0.2724	349.6	0.3000	0.7182
319.85	0.0000	0.3309			
328.05	0.0000	0.4158	306.7	1.0000	0.2102
335.95	0.0000	0.5101	320.0	1.0000	0.3166
345.75	0.0000	0.6498	332.9	1.0000	0.4592
			337.5	1.0000	0.5191
311.1	0.3000	0.2524	343.7	1.0000	0.6110
322.9	0.3000	0.3545			
331.8	0.3000	0.4570			
333.6	0.3000	0.4786			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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, Milwaukee, Wisconsin, USA, was used as received.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
303.35	0.0000	0.0853	304.5	0.3000	0.1702
307.35	0.0000	0.1031	310.3	0.3000	0.2079
312.05	0.0000	0.1274	319.2	0.3000	0.2810
316.45	0.0000	0.1565	326.8	0.3000	0.3602
320.95	0.0000	0.1931			
325.65	0.0000	0.2421	306.7	1.0000	0.2102
329.95	0.0000	0.2984	320.0	1.0000	0.3166
334.65	0.0000	0.3697	332.9	1.0000	0.4592
339.85	0.0000	0.4645	337.5	1.0000	0.5191
346.45	0.0000	0.5992	343.7	1.0000	0.6110
354.45	0.0000	0.7742			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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, Milwaukee, Wisconsin, USA, was used as received.

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

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.1.
$x_3^{(s)}$: $\pm$ 0.0001.
x_1: $\pm$ 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams. C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1
306.55	0.0000	0.2253
312.95	0.0000	0.2724
319.85	0.0000	0.3309
328.05	0.0000	0.4158
335.95	0.0000	0.5101
345.75	0.0000	0.6498
301.5	0.3000	0.2007
309.2	0.3000	0.2514
317.9	0.3000	0.3189
325.7	0.3000	0.3959
335.2	0.3000	0.5039
344.9	0.3000	0.6414
355.6	0.3000	0.8148
307.3	1.0000	0.2548
319.6	1.0000	0.3542
328.4	1.0000	0.4407
335.7	1.0000	0.5224
344.8	1.0000	0.6428

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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, Milwaukee, Wisconsin, USA, was used as received.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
303.35	0.0000	0.0853	321.5	0.3000	0.2820
307.35	0.0000	0.1031	327.8	0.3000	0.3519
312.05	0.0000	0.1274	333.5	0.3000	0.4311
316.45	0.0000	0.1565	340.6	0.3000	0.5381
320.95	0.0000	0.1931	348.0	0.3000	0.6654
325.65	0.0000	0.2421	356.3	0.3000	0.8193
329.95	0.0000	0.2984			
334.65	0.0000	0.3697	307.3	1.0000	0.2584
339.85	0.0000	0.4645	319.6	1.0000	0.3542
346.45	0.0000	0.5992	328.4	1.0000	0.4407
354.45	0.0000	0.7742	335.7	1.0000	0.5224
			344.8	1.0000	0.6428
304.1	0.3000	0.1511			
310.2	0.3000	0.1885			
316.0	0.3000	0.2332			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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, Milwaukee, Wisconsin, USA, was used as received.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, McLaughlin, E.
J. Chem. Eng. Data <u>1985</u>, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data <u>1987</u>, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. <u>1983</u>, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.3	0.0000	0.2584	341.6	0.3000	0.5956
319.6	0.0000	0.3542	350.4	0.3000	0.7258
328.4	0.0000	0.4407			
335.7	0.0000	0.5224	306.7	1.0000	0.2102
344.8	0.0000	0.6428	320.0	1.0000	0.3166
			332.9	1.0000	0.4592
311.5	0.3000	0.2825	337.5	1.0000	0.5191
322.2	0.3000	0.3619	343.7	1.0000	0.6110
331.2	0.3000	0.4572			
335.9	0.3000	0.5195			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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, Milwaukee, Wisconsin, USA, was used as received.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
308.1	0.0000	0.2521	342.6	0.5000	0.5878
312.6	0.0000	0.2849	349.4	0.5000	0.7053
322.2	0.0000	0.3641			
331.9	0.0000	0.4695	300.7	1.0000	0.1239
343.7	0.0000	0.6175	310.9	1.0000	0.1873
351.9	0.0000	0.7461	318.7	1.0000	0.2496
			327.8	1.0000	0.3302
305.6	0.5000	0.2020	336.0	1.0000	0.4477
319.3	0.5000	0.3055	348.3	1.0000	0.6597
328.8	0.5000	0.4065			
336.9	0.5000	0.5046			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

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

(2) 99.6+ %, Aldrich Chemical Company.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

ANTHRACENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

n-hexane + cyclohexane
n-heptane + cyclohexane
n-octane + cyclohexane
2,2,4-trimethylpentane + cyclohexane
cyclohexane + cyclooctane

II. Alkane + Aromatic Hydrocarbon

n-hexane + benzene
n-heptane + benzene
n-octane + benzene
cyclohexane + benzene
methylcyclohexane + benzene
2,2,4-trimethylpentane + benzene
cyclooctane + benzene
n-hexane + methylbenzene
n-heptane + methylbenzene
n-octane + methylbenzene
cyclohexane + methylbenzene
methylcyclohexane + methylbenzene
2,2,4-trimethylpentane + methylbenzene
cyclooctane + methylbenzene
n-hexane + 1,4-dimethylbenzene
n-heptane + 1,4-dimethylbenzene
n-octane + 1,4-dimethylbenzene
cyclohexane + 1,4-dimethylbenzene
methylcyclohexane + 1,4-dimethylbenzene
2,2,4-trimethylpentane + 1,4-dimethylbenzene

III. Alkane + Ester

n-hexane + butyl ethanoate
n-heptane + butyl ethanoate
n-octane + butyl ethanoate
cyclohexane + butyl ethanoate
methylcyclohexane + butyl ethanoate
2,2,4-trimethylpentane + butyl ethanoate
n-hexane + ethyl ethanoate
n-heptane + ethyl ethanoate
n-octane + ethyl ethanoate
cyclohexane + ethyl ethanoate
methylcyclohexane + ethyl ethanoate
2,2,4-trimethylpentane + ethyl ethanoate
n-heptane + dimethyl hexanedioate
cyclohexane + dimethyl hexanedioate
methylcyclohexane + dimethyl hexanedioate
n-hexane + diethyl hexanedioate
n-heptane + diethyl hexanedioate
n-octane + diethyl hexanedioate
cyclohexane + diethyl hexanedioate
methylcyclohexane + diethyl hexanedioate
2,2,4-trimethylpentane + diethyl hexanedioate
n-hexane + dibutyl oxalate

ANTHRACENE SOLUBILITIES (Continued)

n-heptane + dibutyl oxalate
n-octane + dibutyl oxalate
cyclohexane + dibutyl oxalate
methylcyclohexane + dibutyl oxalate
2,2,4-trimethylpentane + dibutyl oxalate

IV. Alkane + Ether

n-hexane + 1,1-oxybisbutane
n-heptane + 1,1-oxybisbutane
n-octane + 1,1-oxybisbutane
cyclohexane + 1,1-oxybisbutane
methylcyclohexane + 1,1-oxybisbutane
n-hexadecane + 1,1-oxybisbutane
2,2,4-trimethylpentane + 1,1-oxybisbutane
cyclooctane + 1,1-oxybisbutane
squalane + 1,1-oxybisbutane
n-hexane + 1,4-dioxane
n-heptane + 1,4-dioxane
n-octane + 1,4-dioxane
cyclohexane + 1,4-dioxane
methylcyclohexane + 1,4-dioxane
2,2,4-trimethylpentane + 1,4-dioxane
cyclooctane + 1,4-dioxane
n-hexane + tetrahydropyran
n-heptane + tetrahydropyran
n-octane + tetrahydropyran
cyclohexane + tetrahydropyran
methylcyclohexane + tetrahydroopyran
2,2,4-trimethylpentane + tetrahydropyran

V. Alkane + Chloroalkane

n-hexane + tetrachloromethane
n-heptane + tetrachloromethane
n-octane + tetrachloromethane
cyclohexane + tetrachloromethane
methylcyclohexane + tetrachloromethane
2,2,4-trimethylpentane + tetracloromethane
n-hexane + 1-chlorobutane
n-heptane + 1-chlorobutane
n-octane + 1-chlorobutane
cyclohexane + 1-chlorobutane
methylcyclohexane + 1-chlorobutane
2,2,4-trimethylpentane + 1-chlorobutane
n-heptane + 1,4-dichlorobutane
n-octane + 1,4-dichlorobutane
cyclohexane + 1,4-dichlorobutane
methylcyclohexane + 1,4-dichlorobutane

VII. Miscellaneous

n-hexane + nitrobenzene
cyclohexane + aniline

ANTHRACENE SOLUBILITIES (Continued)

2,2,4-trimethylpentane + 1-butanol
2,2,4-trimethylpentane + 1-octanol
benzene + trichloromethane
benzene + tetrachloromethane
methylbenzene + tetrachloromethane
1,4-dimethylbenzene + tetrachloromethane
methylbenzene + pyridine
2-propanone + pyridine
2-propanone + nitrobenzene
benzene + methanol
benzene + 1-propanol
methylbenzene + methanol
methylbenzene + phenol
carbon disulfide + 2-propanone
iodoethane + cyclohexene
iodoethane + benzene
iodobenzene + benzene
methanol + carbon disulfide
carbon disulfide + nitrobenzene
nitrobenzene + aniline
bromobenzene + chlorobenzene
benzene + diethyl ether
trichloromethane + diethyl ether

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.001574
0.1735	0.1732	0.001572
0.3565	0.3559	0.001544
0.4498	0.4491	0.001515
0.5571	0.5563	0.001478
0.7646	0.7635	0.001398
1.0000	0.9987	0.001290

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) 99.5+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.001574
0.1542	0.1540	0.001608
0.3283	0.3278	0.001642
0.4230	0.4223	0.001640
0.5250	0.5241	0.001621
0.7236	0.7724	0.001605
0.8813	0.8799	0.001585
1.0000	0.9984	0.001571

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 %, Phillips Petroleum, Bartlesville, Oklahoma, USA.

(3) 99.5+ %, Phillips Petroleum.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.001574
0.1463	0.1461	0.001648
0.3114	0.3109	0.001717
0.3954	0.3948	0.001749
0.5519	0.5509	0.001774
0.7930	0.7915	0.001832
1.0000	0.9982	0.001850

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Chemical Company.

(3) 99.5+ %, Phillips Petroleum Bartlesville, Oklahoma, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.001574
0.1385	0.1383	0.001488
0.2988	0.2984	0.001407
0.3895	0.3890	0.001362
0.5391	0.5384	0.001283
0.7725	0.7716	0.001182
1.0000	0.9989	0.001087

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA.

(3) 99.5+ %, Phillips Petroleum.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.001574
0.1746	0.1743	0.001704
0.3412	0.3406	0.001824
0.4475	0.4467	0.001882
0.5533	0.5522	0.001989
0.7580	0.7564	0.002096
1.0000	0.9977	0.002258

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) 99.5+ %, Phillips Petroleum Bartlesville, Oklahoma, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.007418
0.1442	0.1433	0.006274
0.3093	0.3078	0.004908
0.3842	0.3825	0.004317
0.4963	0.4945	0.003549
0.5536	0.5518	0.003180
0.6624	0.6607	0.002602
0.7365	0.7348	0.002242
1.0000	0.9987	0.001290

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Spectroanalyzed, 99.9+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) Benzene; C_6H_6; [71-43-2]	Acree, W.E., Jr.; Rytting, J.H. *J. Pharm. Sci.* 1983, *72*, 292-296.
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
0.2323	0.2318	0.002283
0.3518	0.3508	0.002783
0.4637	0.4621	0.003375
0.5546	0.5524	0.003922
0.7103	0.7067	0.005022
0.8280	0.8230	0.005987
1.0000	0.9926	0.007418

[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+ %, Phillips Petroleum Bartlesville, Oklahoma, USA.

(3) Spectroanalyzed, 99.9+ %, Fisher Scientific Pittsburgh, Pennsylvania, USA.
Components 2 and 3 were stored over molecular seives 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) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and
S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00742
0.1227	0.1219	0.00616
0.2606	0.2593	0.00508
0.3524	0.3508	0.00444
0.4575	0.4558	0.00377
0.6838	0.6819	0.00280
0.8156	0.8137	0.00239
1.0000	0.9982	0.00184

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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,
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C			*t* = 25.0 °C		
$x_3^{(s),b}$	x_3	x_1	$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00120	0.000	0.000	0.00161
0.341	0.340	0.00267	0.350	0.349	0.00319
0.519	0.517	0.00336	0.518	0.516	0.00420
0.683	0.680	0.00435	0.683	0.679	0.00535
1.000	0.994	0.00616	0.763	0.759	0.00586
			1.000	0.993	0.00711

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavody, 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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, 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	0.001574
0.1731	0.1727	0.002258
0.2320	0.2314	0.002592
0.4380	0.4363	0.003802
0.5427	0.5403	0.004506
0.6357	0.6324	0.005154
0.8317	0.8263	0.006482
1.0000	0.9926	0.007418

[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) 99.5+ %, Phillips Petroleum Bartlesville, Oklahoma, USA.

(3) Spectroanalyzed, 99.9+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA.
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) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00742
0.1519	0.1510	0.00625
0.3209	0.3193	0.00504
0.4098	0.4080	0.00440
0.5257	0.5238	0.00370
0.7353	0.7333	0.00267
0.8716	0.8698	0.00208
1.0000	0.9984	0.00165

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, anhydrous Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

$T/K = 298$, 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	0.001087
0.1601	0.1599	0.001467
0.3127	0.3121	0.001983
0.5398	0.5381	0.003144
0.6354	0.6330	0.003830
0.7209	0.7176	0.004571
0.8591	0.8541	0.005840
1.0000	0.9984	0.007418

[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+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA.

(3) Spectroanalyzed, 99.9+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA.
Components 2 and 3 were stored over molecula 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) Cyclooctane; C_8H_{16}; [292-64-8]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.007418
0.1416	0.1406	0.006814
0.3045	0.3028	0.005708
0.3984	0.3963	0.005282
0.4935	0.4912	0.004745
0.6685	0.6660	0.003740
0.8016	0.7986	0.003069
1.0000	0.9978	0.002258

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) Spectroanalyzed, 99.9+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) Methylbenzene; C_7H_8; [108-88-3]	Tucker, S.A.; Murral, D.J.; Oswalt, B.M.; Halmi, J.L.; Acree, W.E., Jr. *Phys. Chem. Liq.* 1988, *18*, 279-286.
VARIABLES:	**PREPARED BY:**
$T/K = 298$, Solvent composition	W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.1631	0.1621	0.00607
0.3540	0.3524	0.00454
0.4514	0.4496	0.00388
0.5453	0.5435	0.00327
0.7369	0.7352	0.00226
1.0000	0.9987	0.00127

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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.* <u>1988</u>, *18*, 279-286.
VARIABLES: *T*/K = 298, Solvent composition	**PREPARED BY:** W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.1606	0.1596	0.00606
0.1692	0.1682	0.00598
0.3246	0.3230	0.00480
0.3247	0.3232	0.00477
0.4137	0.4120	0.00420
0.4254	0.4236	0.00412
0.5316	0.5298	0.00344
0.5396	0.5378	0.00336
0.7341	0.7323	0.00245
0.7413	0.7395	0.00242
1.0000	0.9984	0.00157

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.9+ %, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** *T*/K: ± 0.05. $x_2^{(s)}$: ± 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) Methylbenzene; C_7H_8; [108-88-3]	Tucker, S.A.; Murral, D.J.; Oswalt, B.M.; Halmi, J.L.; Acree, W.E., Jr. *Phys. Chem. Liq.* 1988, *18*, 279-286.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.1397	0.1388	0.00623
0.1415	0.1406	0.00619
0.2977	0.2962	0.00502
0.3014	0.2999	0.00498
0.3936	0.3919	0.00434
0.4024	0.4007	0.00431
0.4956	0.4937	0.00375
0.4988	0.4969	0.00374
0.7147	0.7128	0.00271
0.7211	0.7192	0.00268
1.0000	0.9982	0.00184

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.2043	0.2031	0.00600
0.3954	0.3935	0.00483
0.4964	0.4943	0.00414
0.5950	0.5929	0.00356
0.7930	0.7910	0.00248
1.0000	0.9984	0.00155

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.1756	0.1745	0.00631
0.1817	0.1806	0.00626
0.3532	0.3514	0.00516
0.3621	0.3603	0.00508
0.4512	0.4492	0.00450
0.4634	0.4613	0.00443
0.5541	0.5520	0.00384
0.5657	0.5636	0.00376
0.7607	0.7586	0.00269
0.7720	0.7700	0.00263
1.0000	0.9984	0.00165

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, anhydrous Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.1362	0.1354	0.00593
0.1381	0.1373	0.00592
0.2926	0.2913	0.00447
0.2944	0.2931	0.00446
0.3895	0.3880	0.00373
0.3921	0.3906	0.00370
0.4862	0.4847	0.00308
0.4932	0.4917	0.00304
0.7059	0.7045	0.00200
0.7127	0.7113	0.00195
1.0000	0.9989	0.00107

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00736
0.1664	0.1653	0.00658
0.3173	0.3155	0.00568
0.4412	0.4390	0.00508
0.5401	0.5377	0.00451
0.7519	0.7494	0.00337
0.9023	0.9973	0.00266
1.0000	0.9977	0.00225

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,4-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00733
0.1945	0.1933	0.00602
0.3807	0.3790	0.00459
0.4823	0.4804	0.00388
0.5882	0.5863	0.00327
0.7833	0.7816	0.00222
0.8619	0.8603	0.00182
1.0000	0.9987	0.00127

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.5+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,4-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00733
0.1747	0.1737	0.00593
0.3547	0.3531	0.00463
0.4490	0.4472	0.00403
0.5571	0.5552	0.00341
0.7648	0.7630	0.00240
0.8836	0.8819	0.00195
1.0000	0.9984	0.00157

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.5+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,4-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00733
0.1631	0.1621	0.00621
0.3491	0.3474	0.00494
0.4395	0.3661	0.00431
0.5346	0.5326	0.00376
0.7454	0.7434	0.00274
0.8678	0.8658	0.00227
1.0000	0.9982	0.00184

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, USA, used as received.

(2) Gold Label, 99+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.5+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,4-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00733
0.2232	0.2218	0.00610
0.4303	0.4282	0.00485
0.5304	0.5282	0.00417
0.6322	0.6300	0.00357
0.8137	0.8117	0.00251
1.0000	0.9984	0.00155

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) HPLC Grade, 99.5+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,4-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00733
0.2045	0.2033	0.00592
0.3822	0.3804	0.00482
0.4879	0.4859	0.00418
0.5939	0.5918	0.00360
0.7977	0.7957	0.00252
0.8578	0.8559	0.00218
1.0000	0.9984	0.00165

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, anhydrous Aldrich Chemical Company.

(3) HPLC Grade, 99.5+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00733
0.1626	0.1617	0.00577
0.3333	0.3319	0.00430
0.4311	0.4296	0.00357
0.5334	0.5318	0.00293
0.7484	0.7470	0.00186
0.8735	0.8723	0.00141
1.0000	0.9989	0.00107

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.5+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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, 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	0.00127
0.1076	0.1074	0.00180
0.2107	0.2057	0.00239
0.3995	0.3981	0.00350
0.4878	0.4858	0.00404
0.5944	0.5916	0.00467
0.7930	0.7885	0.00572
0.8808	0.8754	0.00615
1.0000	0.9934	0.00661

[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-Heptane; C_7H_{16}; [142-82-5]

(3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

J. Chem. Soc., Faraday Trans. <u>1991</u>, *87*, 461-464.

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	0.00157
0.1233	0.1230	0.00218
0.2259	0.2253	0.00275
0.4250	0.4234	0.00387
0.5263	0.5240	0.00446
0.6255	0.6224	0.00501
0.8050	0.9941	0.00586
0.9058	0.9001	0.00629
1.0000	0.9934	0.00661

[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+ %, 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) 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, 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	0.00184
0.1238	0.1235	0.00245
0.2677	0.2668	0.00322
0.4604	0.4584	0.00425
0.5555	0.5528	0.00480
0.6591	0.6556	0.00532
0.8330	0.8280	0.00604
0.9145	0.9087	0.00632
1.0000	0.9934	0.00661

[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) 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, 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	0.00155
0.0948	0.0946	0.00225
0.1704	0.1699	0.00277
0.3559	0.3545	0.00398
0.4493	0.4472	0.00457
0.5268	0.5242	0.00494
0.7596	0.7551	0.00591
0.8694	0.8640	0.00626
1.0000	0.9934	0.00661

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

(3) 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, 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	0.00165
0.1107	0.1104	0.00239
0.2020	0.2014	0.00298
0.3942	0.3926	0.00416
0.4848	0.4825	0.00472
0.5969	0.5938	0.00522
0.7992	0.7943	0.00607
0.8882	0.8826	0.00630
1.0000	0.9934	0.00661

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

(3) 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, 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	0.00107
0.1336	0.1334	0.00158
0.2471	0.2466	0.00211
0.4636	0.4620	0.00332
0.5532	0.5511	0.00385
0.6511	0.6482	0.00447
0.8344	0.8297	0.00565
0.9165	0.9108	0.00617
1.0000	0.9934	0.00661

[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-Hexane; C_6H_{14}; [110-54-3]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00127
0.1336	0.1334	0.00184
0.2498	0.2492	0.00241
0.4557	0.4541	0.00345
0.5662	0.5640	0.00395
0.6627	0.6599	0.00428
0.8395	0.8355	0.00476
0.9192	0.9147	0.00485
1.0000	0.9952	0.00484

[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

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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) 99.5+ %, 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00157
0.1476	0.1473	0.00216
0.2630	0.2623	0.00269
0.4937	0.4918	0.00381
0.5949	0.5924	0.00426
0.6553	0.6524	0.00445
0.8554	0.8511	0.00497
0.9222	0.9177	0.00493
1.0000	0.9952	0.00484

[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+ %, Aldrich Chemical Company.

(3) 99.5+ %, 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00184
0.1616	0.1612	0.00257
0.2990	0.2980	0.00322
0.5243	0.5221	0.00423
0.6128	0.6100	0.00452
0.7155	0.7120	0.00489
0.8746	0.8702	0.00508
0.9378	0.9331	0.00499
1.0000	0.9952	0.00484

[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) 99.5+ %, 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) 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:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00155
0.1178	0.1175	0.00234
0.2320	0.2312	0.00310
0.4266	0.4248	0.00429
0.5274	0.5249	0.00474
0.6296	0.6264	0.00513
0.8150	0.8107	0.00531
0.9051	0.9004	0.00515
1.0000	0.9952	0.00484

[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) 99.5+ %, 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00165
0.1410	0.1406	0.00261
0.2487	0.2479	0.00329
0.4487	0.4468	0.00431
0.5783	0.5755	0.00485
0.6645	0.6611	0.00507
0.8433	0.8389	0.00516
0.9173	0.9127	0.00505
1.0000	0.9952	0.00484

[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

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$x_3^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00107
0.1306	0.1304	0.00147
0.3215	0.3208	0.00221
0.5273	0.5256	0.00313
0.6250	0.6227	0.00362
0.7106	0.7077	0.00402
0.8682	0.8642	0.00465
0.9290	0.9246	0.00477
1.0000	0.9952	0.00484

[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

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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: ± 1.5 % (relative error).

COMPONENTS:

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

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

(3) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00871
0.1193	0.1182	0.00886
0.2222	0.2202	0.00878
0.4328	0.4295	0.00769
0.5267	0.5231	0.00677
0.6199	0.6162	0.00590
0.8179	0.8149	0.00369
0.9072	0.9048	0.00260
1.0000	0.9984	0.00157

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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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ESTIMATED ERRORS:

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$x_2^{(s)}$: ± 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) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00871
0.1561	0.1547	0.00889
0.2940	0.2914	0.00872
0.4992	0.4954	0.00765
0.6047	0.6006	0.00676
0.7014	0.6974	0.00572
0.8569	0.8537	0.00368
0.9235	0.9213	0.00268
1.0000	0.9984	0.00155

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

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$x_2^{(s)}$: ± 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]

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ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

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EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00871
0.1295	0.1283	0.00898
0.2415	0.2394	0.00888
0.4605	0.4569	0.00789
0.5686	0.5646	0.00697
0.6674	0.6634	0.00596
0.8357	0.8324	0.00393
0.9100	0.9073	0.00295
1.0000	0.9984	0.00165

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ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

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

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

(3) Diethyl hexanedioate; $C_{10}H_{18}O_4$; [141-28-6]

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. <u>1991</u>, *24*, 31-42.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00127
0.0624	0.0623	0.00199
0.1414	0.1410	0.00296
0.3032	0.3017	0.00482
0.3960	0.3937	0.00591
0.4999	0.4964	0.00699
0.7181	0.7117	0.00887
0.8282	0.8203	0.00952
1.0000	0.9897	0.01033

[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.

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ORIGINAL MEASUREMENTS:

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00157
0.0887	0.0885	0.00254
0.1544	0.1539	0.00328
0.3278	0.3261	0.00522
0.4176	0.4150	0.00619
0.5344	0.5305	0.00735
0.7352	0.7286	0.00896
0.8621	0.8538	0.00962
1.0000	0.9897	0.01033

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COMPONENTS:

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

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

(3) Diethyl hexanedioate; $C_{10}H_{18}O_4$; [141-28-6]

ORIGINAL MEASUREMENTS:

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

VARIABLES:

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EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00184
0.0868	0.0866	0.00280
0.1721	0.1715	0.00377
0.3402	0.3383	0.00567
0.4447	0.4417	0.00679
0.5480	0.5437	0.00776
0.6732	0.6673	0.00877
0.8715	0.8629	0.00989
1.0000	0.9897	0.01033

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t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00155
0.0611	0.0610	0.00245
0.1187	0.1183	0.00327
0.2661	0.2647	0.00511
0.3541	0.3519	0.00616
0.4508	0.4476	0.00716
0.6832	0.6771	0.00886
0.8279	0.8200	0.00952
1.0000	0.9952	0.01033

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EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00165
0.0682	0.0680	0.00258
0.1344	0.1339	0.00344
0.2960	0.2944	0.00540
0.3889	0.3864	0.00645
0.4862	0.4826	0.00731
0.6317	0.6263	0.00856
0.8405	0.8324	0.00967
1.0000	0.9897	0.01033

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COMPONENTS:

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

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VARIABLES:

T/K = 298, Solvent composition

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EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00107
0.0894	0.0892	0.00182
0.1723	0.1718	0.00264
0.3411	0.3396	0.00443
0.4555	0.4529	0.00565
0.5626	0.5588	0.00678
0.7615	0.7549	0.00865
0.8684	0.8602	0.00949
1.0000	0.9897	0.01033

[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.

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(3) 99 %, 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-Hexane; C_6H_{14}; [110-54-3]

(3) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01043
0.1575	0.1560	0.00965
0.2995	0.2970	0.00850
0.5129	0.5096	0.00648
0.6130	0.6096	0.00551
0.6999	0.6967	0.00456
0.8623	0.8599	0.00277
0.9293	0.9274	0.00201
1.0000	0.9987	0.00127

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shorlty before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01043
0.1459	0.1445	0.00959
0.2630	0.2607	0.00881
0.4833	0.4799	0.00694
0.5799	0.5764	0.00597
0.6797	0.6763	0.00498
0.8500	0.8473	0.00313
0.9195	0.9173	0.00240
1.0000	0.9984	0.00157

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

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SOURCE AND PURITY OF MATERIALS:

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(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01043
0.1164	0.1152	0.00991
0.2387	0.2365	0.00915
0.4527	0.4494	0.00734
0.5566	0.5530	0.00646
0.6628	0.6592	0.00542
0.8339	0.8309	0.00364
0.9114	0.9089	0.00275
1.0000	0.9982	0.00184

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01043
0.1683	0.1667	0.00957
0.3317	0.3288	0.00860
0.5625	0.5587	0.00673
0.6557	0.6519	0.00579
0.7420	0.7384	0.00484
0.8818	0.8790	0.00314
0.9402	0.9380	0.00235
1.0000	0.9984	0.00155

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01043
0.1702	0.1686	0.00960
0.2855	0.2830	0.00880
0.5185	0.5149	0.00702
0.6203	0.6165	0.00606
0.7115	0.7078	0.00514
0.8603	0.8573	0.00346
0.9196	0.9176	0.00217
1.0000	0.9984	0.00165

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01043
0.1279	0.1267	0.00941
0.2522	0.2501	0.00832
0.4556	0.4527	0.00627
0.5538	0.5509	0.00531
0.6501	0.6473	0.00436
0.8312	0.8291	0.00258
0.9151	0.9135	0.00180
1.0000	0.9989	0.00107

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2515	0.2508	0.002944
0.4505	0.4494	0.002453
0.4516	0.4505	0.002444
0.5676	0.5664	0.002177
0.6493	0.6480	0.001989
0.6501	0.6488	0.001979
0.8402	0.8389	0.001571
1.0000	0.9987	0.001273

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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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) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,1-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2330	0.2323	0.003091
0.4186	0.4175	0.002676
0.4200	0.4189	0.002647
0.5379	0.5366	0.002447
0.6243	0.6229	0.002258
0.8130	0.8115	0.001894
1.0000	0.9984	0.001568

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, USA, used as received.

(2) HPLC Grade, 99+ %, Aldrich Chemical Company.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,1-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2167	0.2160	0.003185
0.4059	0.4047	0.002837
0.5116	0.5102	0.002652
0.6030	0.6015	0.002478
0.7914	0.7897	0.002151
1.0000	0.9982	0.001836

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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SOURCE AND PURITY OF MATERIALS:

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(2) Gold Label, 99+ %, Aldrich Chemical Company.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1,1-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2869	0.2860	0.003066
0.5080	0.5067	0.002647
0.6074	0.6059	0.002435
0.7032	0.7016	0.002230
0.8577	0.8561	0.001884
0.8591	0.8575	0.001867
1.0000	0.9984	0.001551

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

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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) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

$x_2^{(s)}$: ± 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) 1,1-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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2544	0.2536	0.003122
0.4391	0.4379	0.002799
0.5727	0.5713	0.002520
0.5738	0.5724	0.002511
0.6674	0.6659	0.002315
0.8201	0.8184	0.002021
0.8228	0.8211	0.002009
1.0000	0.9983	0.001652

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00380
0.1328	0.1323	0.00376
0.2139	0.2131	0.00372
0.3046	0.3035	0.00370
0.3963	0.3948	0.00370
0.4844	0.4826	0.00368
0.5811	0.5790	0.00367
0.7051	0.7025	0.00368
0.7993	0.7964	0.00365
0.8887	0.8855	0.00360
1.0000	0.9965	0.00354

[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 tetrachloromethane. Concentrations were 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, used as received.

(3) Gold Label, 99+ %, Aldrich Chemical Company, was 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) 1,1-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, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00660	1.202	0.00849
0.01088	0.00636	1.498	0.00918
0.0299	0.00627	1.998	0.0101
0.0495	0.00639	3.031	0.0127
0.0847	0.00637	3.983	0.0153
0.1246	0.00646	4.763	0.0174
0.4216	0.00704	5.867	0.0210
0.6936	0.00749		
0.8675	0.00792		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, used as received.

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

(3) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
$c_3^{(s)}$ four significant figures (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2142	0.2136	0.002942
0.4073	0.4063	0.002391
0.5008	0.4997	0.002146
0.6114	0.6103	0.001860
0.7886	0.7874	0.001469
0.8831	0.8820	0.001280
1.0000	0.9989	0.001067

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

$x_2^{(s)}$: ± 0.0001.

x_1: ± 1 % (relative error).

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.003609
0.2387	0.2379	0.003481
0.4663	0.4648	0.003242
0.5512	0.5495	0.003114
0.6522	0.6503	0.002961
0.8273	0.8251	0.002653
1.0000	0.9977	0.002251

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

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

(2) 2,6,10,15,19,23-Hexamethyltetracosane; $C_{30}H_{62}$; [111-01-3]

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00472
0.1589	0.1582	0.00439
0.2667	0.2656	0.00424
0.4445	0.4427	0.00396
0.5711	0.5689	0.00385
0.6675	0.6650	0.00375
0.7560	0.7532	0.00368
0.8169	0.8139	0.00366
0.9019	0.8986	0.00361
1.0000	0.9965	0.00354

[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 tetrachloromethane. Concentrations were 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, used as received.

(3) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before 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) 1,4-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. <u>1987</u>, *76*, 621-626.

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	0.001273
0.1503	0.1500	0.002216
0.2837	0.2828	0.003292
0.5034	0.5007	0.005325
0.5089	0.5062	0.005381
0.6036	0.5997	0.006383
0.6044	0.6005	0.006438
0.6953	0.6902	0.007337
0.6988	0.6936	0.007371
0.8581	0.8508	0.008562
0.8615	0.8541	0.008563
1.0000	0.9916	0.008381

[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:

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

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

(3) 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, 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	0.001568
0.1573	0.1569	0.002482
0.3048	0.3037	0.003610
0.5286	0.5256	0.005723
0.6381	0.6338	0.006797
0.7181	0.7127	0.007586
0.8733	0.8659	0.008482
1.0000	0.9916	0.008381

[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+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.8 %, Aldrich Chemical Company.

Components 2 and 3 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) 1,4-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, 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	0.001836
0.1841	0.1836	0.002903
0.3295	0.3282	0.004040
0.5568	0.5534	0.006131
0.6555	0.6509	0.007042
0.7432	0.7374	0.007808
0.8813	0.8735	0.008815
0.9406	0.9326	0.008519
1.0000	0.9916	0.008381

[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) Gold Label, 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:

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

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

(3) 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, 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	0.001551
0.1338	0.1334	0.002676
0.2471	0.2461	0.003883
0.4557	0.4529	0.006194
0.5574	0.5534	0.007125
0.6580	0.6527	0.008052
0.7381	0.7319	0.008408
0.8399	0.8323	0.009073
0.9087	0.9008	0.008688
1.0000	0.9916	0.008381

[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) 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) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	Procyk, A.D.; Bissell, M.; Street, K.W., Jr.; Acree, W.E., Jr. *J. Pharm. Sci.* 1987, *76*, 621-626.
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	0.001652
0.1425	0.1421	0.002799
0.2660	0.2650	0.003913
0.5008	0.4977	0.006250
0.5999	0.5956	0.007165
0.6912	0.6857	0.007937
0.7712	0.7647	0.008466
0.8529	0.8454	0.008813
0.9205	0.9125	0.008640
1.0000	0.9916	0.008381

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

(3) 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, 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	0.001067
0.1886	0.1882	0.001927
0.3320	0.3310	0.002891
0.5566	0.5539	0.004903
0.6594	0.6555	0.005988
0.7491	0.7439	0.006942
0.8850	0.8778	0.008121
1.0000	0.9916	0.008381

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

(3) 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, 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	0.002251
0.1497	0.1492	0.003654
0.2855	0.2840	0.005122
0.5078	0.5040	0.007462
0.6128	0.6077	0.008338
0.7008	0.6946	0.008896
0.7842	0.7769	0.009281
0.8580	0.8500	0.009339
0.9329	0.9246	0.008893
1.0000	0.9916	0.008381

[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 equilibrim 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) Gold Label, 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:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01024
0.1507	0.1495	0.00781
0.3320	0.3301	0.00568
0.4242	0.4222	0.00474
0.5194	0.5173	0.00397
0.7431	0.7413	0.00243
0.8686	0.8670	0.00175
1.0000	0.9987	0.00127

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 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.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01024
0.1472	0.1460	0.00786
0.3076	0.3058	0.00593
0.3970	0.3950	0.00499
0.5001	0.4980	0.00411
0.7269	0.7609	0.00262
0.8551	0.8533	0.00207
1.0000	0.9984	0.00157

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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+ %, Aldrich Chemical Chemical Company.

(3) Gold Label, 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.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01024
0.1409	0.1398	0.00794
0.2829	0.2812	0.00614
0.3801	0.3781	0.00521
0.4727	0.4706	0.00444
0.7030	0.7009	0.00300
0.8344	0.8324	0.00237
1.0000	0.9982	0.00184

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, Aldrich Chemical Company.

(3) Gold Label, 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.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01024
0.1875	0.1860	0.00806
0.3767	0.3744	0.00601
0.3824	0.3801	0.00595
0.4685	0.4661	0.00515
0.4766	0.4742	0.00511
0.5738	0.5714	0.00424
0.5752	0.5728	0.00422
0.7795	0.7774	0.00272
0.8797	0.8778	0.00215
1.0000	0.9984	0.00155

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 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.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01024
0.1666	0.1653	0.00806
0.3274	0.3254	0.00626
0.4336	0.4313	0.00527
0.5517	0.5493	0.00427
0.7467	0.7445	0.00295
0.8693	0.8673	0.00229
1.0000	0.9984	0.00165

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company.

(3) Gold Label, 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.
$x_2^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01024
0.1398	0.1388	0.00738
0.2860	0.2845	0.00525
0.3731	0.3715	0.00429
0.4556	0.4540	0.00360
0.6893	0.6878	0.00211
0.8380	0.8368	0.00148
1.0000	0.9989	0.00107

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 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.

$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00464
0.1585	0.1579	0.00378
0.3229	0.3219	0.00299
0.4318	0.4307	0.00257
0.5303	0.5291	0.00226
0.7356	0.7343	0.00176
0.8631	0.8618	0.00150
1.0000	0.9987	0.00127

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) Tetrachloromethane; CCl_4; [56-23-5]	Tucker, S.A.; Acree, W.E., Jr. *Phys. Chem. Liq.* 1989, *19*, 73-79.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00464
0.1492	0.1486	0.00380
0.3062	0.3052	0.00311
0.3935	0.3924	0.00281
0.4941	0.4929	0.00250
0.7096	0.7082	0.00201
0.8448	0.8433	0.00178
1.0000	0.9984	0.00157

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) Tetrachloromethane; CCl_4; [56-23-5]	Tucker, S.A.; Acree, W.E., Jr. *Phys. Chem. Liq.* <u>1989</u>, *19*, 73-79.
VARIABLES:	**PREPARED BY:**
$T/K = 298$, Solvent composition	W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00464
0.1343	0.1338	0.00392
0.2818	0.2809	0.00330
0.3672	0.3661	0.00302
0.4743	0.4730	0.00268
0.6934	0.6918	0.00225
0.8407	0.8390	0.00205
1.0000	0.9982	0.00184

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, USA, used as received.

(2) Gold Label, 99+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S. A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00464
0.1847	0.1840	0.00387
0.3702	0.3690	0.00318
0.4715	0.4702	0.00285
0.5722	0.5707	0.00254
0.8245	0.8229	0.00191
1.0000	0.9984	0.00155

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

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

(2) Methylcyclohexane; C_7H_{16}; [108-87-2]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00464
0.1921	0.1914	0.00373
0.3341	0.3330	0.00318
0.4282	0.4270	0.00289
0.5316	0.5302	0.00262
0.7452	0.7436	0.00212
0.8536	0.8520	0.00190
1.0000	0.9983	0.00165

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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) Gold Label, 99+ %, anhydrous Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

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

(2) 2,2,4-Trimethylpentane; C_7H_{16}; [540-84-1]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00464
0.1069	0.1065	0.00379
0.2791	0.2783	0.00285
0.3652	0.3643	0.00249
0.4633	0.4623	0.00214
0.6890	0.6879	0.00157
0.8367	0.8356	0.00130
1.0000	0.9989	0.00107

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 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) 1-Chlorobutane; C_4H_9Cl; [109-63-3]	Acree, W.E., Jr. *J. Solution Chem.* 1991, *20*, 307-318.
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	0.00127
0.1296	0.1294	0.00165
0.2389	0.2384	0.00204
0.4512	0.4499	0.00290
0.5521	0.5502	0.00340
0.6629	0.6603	0.00399
0.8358	0.8316	0.00497
0.9211	0.9161	0.00538
1.0000	0.9941	0.00586

[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, 99.5+ %, 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) n-Heptane; C_7H_{16}; [142-82-5] (3) 1-Chlorobutane; C_4H_9Cl; [109-63-3]	Acree, W.E., Jr. *J. Solution Chem.* 1991, *20*, 307-318.
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	0.00157
0.1537	0.1534	0.00200
0.2705	0.2699	0.00240
0.4799	0.4784	0.00322
0.5860	0.5838	0.00370
0.6737	0.6709	0.00415
0.8489	0.8447	0.00500
0.9235	0.9185	0.00542
1.0000	0.9941	0.00586

[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+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.5+ %, 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) n-Octane; C_8H_{18}; [111-65-9] (3) 1-Chlorobutane; C_4H_9Cl; [109-63-3]	Acree, W.E., Jr. *J. Solution Chem.* 1991, *20*, 307-318.
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	0.00184
0.1632	0.1628	0.00230
0.2815	0.2807	0.00267
0.5035	0.5017	0.00348
0.6092	0.6068	0.00390
0.7039	0.7008	0.00435
0.8602	0.8558	0.00510
0.9200	0.9150	0.00539
1.0000	0.9941	0.00586

[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, 99.5+ %, 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) 1-Chlorobutane; C_4H_9Cl; [109-63-3]	Acree, W.E., Jr. *J. Solution Chem.* <u>1991</u>, *20*, 307-318.
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	0.00155
0.1091	0.1089	0.00204
0.2094	0.2089	0.00253
0.4108	0.4094	0.00343
0.5124	0.5104	0.00393
0.6140	0.6113	0.00442
0.7964	0.7923	0.00516
0.8935	0.8886	0.00550
1.0000	0.9941	0.00586

[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) HPLC Grade, 99.5+ %, 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) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 1-Chlorobutane; C_4H_9Cl; [109-63-3]	Acree, W.E., Jr. *J. Solution Chem.* 1991, *20*, 307-318.
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	0.00165
0.1308	0.1305	0.00216
0.2359	0.2353	0.00261
0.4352	0.4337	0.00345
0.5379	0.5358	0.00390
0.6420	0.6392	0.00436
0.8161	0.8120	0.00508
0.9170	0.9119	0.00556
1.0000	0.9941	0.00586

[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) Gold Label, 99+ % anhydrous, Aldrich Chemical Company.

(3) HPLC Grade, 99.5+ %, 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-Chlorobutane; C_4H_9Cl; [109-63-3]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

J. Solution Chem. 1991, *20*, 307-318.

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	0.00107
0.1490	0.1488	0.00142
0.2874	0.2869	0.00183
0.5109	0.5095	0.00270
0.6145	0.6125	0.00320
0.6940	0.6914	0.00368
0.8546	0.8505	0.00478
0.9322	0.9272	0.00532
1.0000	0.9941	0.00586

[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, 99.5+ %, 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) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1991, *23*, 225-237.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00157
0.1379	0.1375	0.00276
0.2507	0.2497	0.00392
0.4470	0.4442	0.00625
0.5682	0.5638	0.00768
0.6581	0.6524	0.00873
0.8425	0.8339	0.01026
0.9120	0.9024	0.01049
1.0000	0.9895	0.01053

[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, was used as received.

(2) HPLC Grade, 99+ %, Aldrich Chemical Company.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 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) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1991, *23*, 225-237.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00184
0.1528	0.1523	0.00312
0.2670	0.2659	0.00430
0.4983	0.4948	0.00697
0.5934	0.5886	0.00807
0.6854	0.6792	0.00911
0.8550	0.8461	0.01041
0.9254	0.9157	0.01051
1.0000	0.9895	0.01053

[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) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.05.
$x_3^{(s)}$: $\pm$ 0.0001.
x_1: $\pm$ 1.5 % (relative error).

COMPONENTS:

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

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

(3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1991, *23*, 225-237.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00155
0.1066	0.1063	0.00278
0.1993	0.1985	0.00394
0.3903	0.3878	0.00638
0.4994	0.4956	0.00754
0.5985	0.5934	0.00854
0.7962	0.7883	0.00987
0.8837	0.8747	0.01023
1.0000	0.9895	0.01053

[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, was used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1991, *23*, 225-237.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00165
0.1237	0.1233	0.00294
0.2298	0.2288	0.00417
0.4314	0.4286	0.00646
0.5259	0.5219	0.00761
0.6270	0.6216	0.00859
0.8192	0.8110	0.00996
0.8998	0.8905	0.01035
1.0000	0.9895	0.01053

[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) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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-Hexane; C_6H_{14}; [110-54-3]

(3) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0103
0.134	0.133	0.0109
0.365	0.361	0.0100
0.542	0.538	0.0077
0.795	0.792	0.0039
1.000	0.999	0.0015

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

(3) Aniline; C_6H_7N; [62-53-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 313, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 40 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0077
0.267	0.265	0.0089
0.508	0.503	0.0094
0.813	0.809	0.0048
1.000	0.997	0.0031

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

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:

Anderson, B.D.

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00660	2.370	0.00859
0.03705	0.00692	2.953	0.00867
0.0806	0.00698	3.950	0.00892
0.1191	0.00723	5.992	0.00935
0.2014	0.00723	7.913	0.00936
0.3960	0.00752	9.302	0.00954
0.6170	0.00799	10.87	0.00950
0.8248	0.00805		
1.298	0.00813		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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.

(3) puriss, 99.5 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
$c_3^{(s)}$: 4 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

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:

Anderson, B.D.

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00660	1.033	0.00833
0.03897	0.00656	1.970	0.00994
0.08065	0.00689	2.958	0.0111
0.1226	0.00693	3.941	0.0120
0.2120	0.00717	4.997	0.0129
0.4360	0.00738	6.313	0.0140
0.6914	0.00819		
0.778	0.00850		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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.

(3) 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: $\pm$ 0.1 (compiler).

$c_3^{(s)}$: 4 sig. figs. (compiler).

c_1: $\pm$ 3 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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 = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00711
0.179	0.178	0.00723
0.247	0.245	0.00724
0.396	0.393	0.00739
0.566	0.562	0.00775
0.663	0.657	0.00837
0.840	0.832	0.00945
1.000	0.990	0.0105

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavody, 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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 and 298,
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C			t = 25.0 °C		
$x_3^{(s),b}$	x_3	x_1	$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00595	0.000	0.000	0.00711
0.202	0.201	0.00570	0.202	0.201	0.00693
0.336	0.334	0.00564	0.336	0.334	0.00662
0.504	0.501	0.00531	0.504	0.501	0.00622
0.604	0.601	0.00545	0.604	0.600	0.00603
1.000	0.996	0.00411	1.000	0.995	0.00483

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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, 313 and 333,
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00645
0.166	0.165	0.00595
0.375	0.373	0.00565
0.642	0.639	0.00505
1.000	0.996	0.00411

t = 40.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.0124
0.166	0.164	0.0119
0.375	0.371	0.0110
0.641	0.635	0.00977
1.000	0.992	0.00836

t = 60.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.0230
0.062	0.061	0.0220
0.166	0.162	0.0217
0.285	0.279	0.0212
0.375	0.367	0.0209
0.473	0.464	0.0200
0.642	0.630	0.0188
0.846	0.832	0.0169
1.000	0.984	0.0156

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavody, 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
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]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00770
0.256	0.254	0.00752
0.408	0.405	0.00694
0.580	0.576	0.00611
1.000	0.995	0.00483

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.05.
x_3: $\pm$ 0.001 (compiler).
x_1: $\pm$ 3 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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,
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C			t = 60.0 °C		
$x_3^{(s),b}$	x_3	x_1	$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00645	0.000	0.000	0.0230
0.115	0.114	0.00736	0.225	0.219	0.0260
0.279	0.277	0.00825	0.279	0.271	0.0271
0.437	0.433	0.00856	0.437	0.425	0.0281
0.538	0.533	0.00863	0.538	0.523	0.0287
0.636	0.630	0.00895	0.636	0.617	0.0293
0.777	0.770	0.00880	0.731	0.709	0.0297
0.823	0.816	0.00875	0.823	0.799	0.0288
1.000	0.992	0.00834	1.000	0.972	0.0284

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavody, 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

(2) 2-Propanone; C_3H_6O; [67-64-1]

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00834
0.312	0.310	0.00702
0.576	0.573	0.00560
0.803	0.800	0.00431
1.000	0.997	0.00313

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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(1) 95 % initial purity, Urxovy Zavody, 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
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]

(3) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0103
0.413	0.409	0.0092
0.657	0.652	0.0069
0.861	0.857	0.0051
1.000	0.996	0.0043

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25\ ^\circ C$

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.00025
0.124	0.124	0.00072
0.303	0.303	0.00175
0.539	0.537	0.00398
0.751	0.747	0.00569
1.000	0.993	0.00740

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.5 (compiler).
$x_2^{(s)}$: $\pm$ 0.001 (compiler).
x_1: $\pm$ 5 % (relative error; compiler).

COMPONENTS:

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

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

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.00037
0.229	0.229	0.00140
0.444	0.443	0.00290
0.687	0.684	0.00457
1.000	0.993	0.00740

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00645
0.242	0.241	0.00509
0.489	0.487	0.00395
0.657	0.656	0.00193
0.742	0.741	0.00136
0.812	0.811	0.000948
0.897	0.896	0.000570
0.963	0.963	0.000288
1.000	1.000	0.000202

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

(2) Phenol; C_6H_6O; [108-95-2]

(3) 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 = 313, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 40.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.0124
0.246	0.243	0.0113
0.495	0.490	0.00940
0.746	0.741	0.00715
1.000	0.995	0.00487

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavody, 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

(2) Carbon disulfide; CS_2; [75-15-0]

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00872
0.247	0.244	0.0108
0.304	0.301	0.0109
0.360	0.356	0.0108
0.466	0.461	0.0101
0.567	0.562	0.00913
0.797	0.792	0.00595
1.000	0.997	0.00313

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

(2) Iodoethane; C_2H_5I; [74-88-4]

(3) Cyclohexene; C_6H_{10}; [110-83-8]

ORIGINAL MEASUREMENTS:

Somayajulu, G.R.; Palit, S.R.

J. Phys. Chem. 1954, *58*, 417-421.

VARIABLES:

T/K = 310, 320 and 330
Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 37 °C			t = 57 °C		
$x_3^{(s)}$	x_3[b]	x_1	$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.01189	0.0000	0.0000	0.02175
0.1117	0.1104	0.01161	0.1117	0.1090	0.02455
0.2128	0.2104	0.01117	0.2128	0.2078	0.02344
0.4765	0.4724	0.00859	0.4765	0.4678	0.01820
0.5451	0.5410	0.00759	0.5451	0.5361	0.01660
1.0000	0.9954	0.00457	1.0000	0.9902	0.00977

t = 47 °C		
0.0000	0.0000	0.01612
0.1117	0.1098	0.01708
0.2128	0.2093	0.01641
0.4765	0.4705	0.01259
0.5451	0.5389	0.01143
1.0000	0.9933	0.00668

[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 mixture.

[b] computed by compiler.

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 0.5 K per minute. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. To verify the experimental solubilities, the cloud-point temperature was also determined. Reported values were computed from the variation of mole fraction solubility as a function of solution temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, J.T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate.

(2) Purity not specified, Eastman Kodak Chemical Company, USA, was dried over calcium chloride and distilled shortly before use.

(3) AR Grade, thiophene free, source not specified, was dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3.
$x_3^{(s)}$: ± 0.0001 (compiler).
x_1: ± 0.00001 (compiler).

COMPONENTS:

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

(2) Iodoethane; C_2H_5I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

Somayajulu, G.R.; Palit, S.R.

J. Phys. Chem. 1954, *58*, 417-421.

VARIABLES:

T/K = 310, 320, 330 and 340
Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 37 °C

$x_3^{(s)}$	x_3^{b}	x_1
0.0000	0.0000	0.01189
0.3306	0.3263	0.01303
0.4780	0.4716	0.01342
0.5721	0.5646	0.01303
0.7083	0.6997	0.01216
1.0000	0.9894	0.01059

t = 47 °C

$x_3^{(s)}$	x_3^{b}	x_1
0.0000	0.0000	0.01612
0.3306	0.3247	0.01778
0.4780	0.4693	0.01820
0.5721	0.5619	0.01778
0.7083	0.6965	0.01660
1.0000	0.9856	0.01437

t = 57 °C

$x_3^{(s)}$	x_3^{b}	x_1
0.0000	0.0000	0.02175
0.3306	0.3227	0.02385
0.4780	0.4664	0.02435
0.5721	0.5585	0.02385
0.7083	0.6925	0.02226
1.0000	0.9807	0.01934

t = 67 °C

$x_3^{(s)}$	x_3^{b}	x_1
0.0000	0.0000	0.02867
0.3306	0.3202	0.03141
0.4780	0.4626	0.03219
0.5721	0.5541	0.03141
0.7083	0.6874	0.02951
1.0000	0.9744	0.02558

[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 mixture.

[b] computed by compiler.

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 0.5 K per minute. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. To verify the experimental solubilities, the cloud-point temperature was also determined. Reported values were computed from the variation of mole fraction solubility as a function of solution temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, J.T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate.

(2) Purity not specified, prepared by the authors, dried over calcium chloride and distilled before use.

(3) AR Grade, thiophene free, source not specified, was dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3.
$x_3^{(s)}$: ± 0.0001 (compiler).
x_1: ± 0.00001 (compiler).

COMPONENTS:

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

(2) Iodobenzene; C_6H_5I; [591-50-4]

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

ORIGINAL MEASUREMENTS:

Somayajulu, G.R.; Palit, S.R.

J. Phys. Chem. 1954, *58*, 417-421.

VARIABLES:

T/K = 305, 310, 315, 320, 325 and 330, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 32 °C			t = 42 °C		
$x_3^{(s)}$	x_3^{b}	x_1	$x_3^{(s)}$	x_3^{b}	x_1
0.0000	0.0000	0.01462	0.0000	0.0000	0.02014
0.0639	0.0629	0.01622	0.0639	0.0625	0.02213
0.1917	0.1886	0.01622	0.1917	0.1875	0.02213
0.3459	0.3406	0.01549	0.3459	0.3386	0.02113
0.5615	0.5538	0.01365	0.5615	0.5510	0.01862
1.0000	0.9909	0.00912	1.0000	0.9876	0.01245
t = 37 °C			t = 47 °C		
0.0000	0.0000	0.01728	0.0000	0.0000	0.02344
0.0639	0.0627	0.01916	0.0639	0.0623	0.02570
0.1917	0.1880	0.01916	0.1917	0.1868	0.02570
0.3459	0.3396	0.01820	0.3459	0.3374	0.02469
0.5615	0.5525	0.01594	0.5615	0.5493	0.02175
1.0000	0.9894	0.01059	1.0000	0.9856	0.01437

(Continued next page)

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 0.5 K per minute. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. To verify the experimental solubilities, the cloud-point temperature was also determined. Reported values were computed from the variation of mole fraction solubility as a function of solution temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, J.T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate.

(2) Purity not specified, Columbia Organic Chemicals, USA, was distilled before use.

(3) AR Grade, thiophene free, source not specified, was dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3.
$x_3^{(s)}$: ± 0.0001 (compiler).
x_1: ± 0.00001 (compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Iodobenzene; C_6H_5I; [591-50-4] (3) Benzene; C_6H_6; [71-43-2]	Somayajulu, G.R.; Palit, S.R. *J. Phys. Chem.* 1954, *58*, 417-421.
VARIABLES:	**PREPARED BY:**
T/K = 305, 310, 315, 320, 325 and 330, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 52 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.02738
0.0639	0.0620	0.03002
0.1917	0.1859	0.03002
0.3459	0.3360	0.02867
0.5615	0.5473	0.02526
1.0000	0.9830	0.01698

t = 57 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.03145
0.0639	0.0617	0.03447
0.1917	0.1851	0.03447
0.3459	0.3345	0.03293
0.5615	0.5452	0.02900
1.0000	0.9807	0.01934

[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 mixture.

[b] computed by compiler.

COMPONENTS:

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

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

(3) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

$T/K = 313$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 40\ °C$

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0132
0.454	0.452	0.00473
0.663	0.662	0.00198
0.881	0.880	0.00097
1.000	0.999	0.00030

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.5 (compiler).
$x_2^{(s)}$: $\pm$ 0.001 (compiler).
x_1: $\pm$ 5 % (relative error; compiler).

COMPONENTS:

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

(2) Carbon disulfide; CS_2; [75-15-0]

(3) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0103
0.379	0.375	0.0111
0.626	0.618	0.0132
0.836	0.823	0.0156
1.000	0.991	0.0086

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (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]

(3) Aniline; C_6H_7N; [62-53-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25$ °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0039
0.270	0.268	0.0073
0.442	0.438	0.0097
0.726	0.709	0.0229
1.000	0.990	0.0103

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) Bromobenzene; C_6H_6Br; [108-86-1]

(3) Chlorobenzene; C_7H_8Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0102
0.189	0.187	0.0105
0.413	0.408	0.0110
0.688	0.680	0.0114
1.000	0.988	0.0119

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

(3) Diethyl ether; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0035
0.287	0.286	0.0042
0.487	0.484	0.0054
0.695	0.691	0.0062
1.000	0.993	0.0074

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

(3) Diethyl ether; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25$ °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.0035
0.205	0.203	0.0029
0.305	0.304	0.0030
0.636	0.633	0.0046
1.000	0.989	0.0107

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 5 % (relative error; compiler).

BIPHENYL SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

cyclohexane + n-hexane
cyclohexane + n-heptane
cyclohexane + n-octane

II. Alkane + Aromatic Hydrocarbon

cyclohexane + benzene

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

n-hexane + tetrachloromethane
n-heptane + tetrachloromethane
cyclohexane + tetrachloromethane

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + thiophene
cyclohexane + thiophene
benzene + pyridine
cyclohexane + pyridine
pyridine + thiophene
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.1233
0.2134	0.1840	0.1378
0.3618	0.3084	0.1476
0.5311	0.4456	0.1609
0.6844	0.5662	0.1727
0.8179	0.6693	0.1817
1.0000	0.8079	0.1921

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Company, Milwaukee, Wisconsin, USA, lized 3 times from methanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company.

(3) 99 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.1381
0.1831	0.1561	0.1477
0.3654	0.3080	0.1571
0.5455	0.4548	0.1663
0.7386	0.6082	0.1765
0.8511	0.6941	0.1845
1.0000	0.8079	0.1921

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) 99+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.1480
0.1463	0.1238	0.1539
0.3314	0.2783	0.1601
0.5016	0.4176	0.1675
0.7318	0.6009	0.1789
0.8293	0.6779	0.1825
1.0000	0.8079	0.1921

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
302.35	0.0000	0.2348	323.55	0.5000	0.6672
310.45	0.0000	0.3540	324.95	0.5000	0.6953
314.65	0.0000	0.4319			
320.85	0.0000	0.5616	290.25	0.7000	0.2843
326.95	0.0000	0.6929	300.85	0.7000	0.3846
333.05	0.0000	0.8252	306.75	0.7000	0.4484
			314.55	0.7000	0.5491
297.05	0.3000	0.2704	323.55	0.7000	0.6784
302.95	0.3000	0.3361			
309.05	0.3000	0.4182	307.95	1.0000	0.4833
313.35	0.3000	0.4857	313.85	1.0000	0.5561
319.45	0.3000	0.5826	316.85	1.0000	0.5932
325.95	0.3000	0.6990	323.65	1.0000	0.6897
			328.95	1.0000	0.7711
290.45	0.5000	0.2524	333.15	1.0000	0.8422
298.65	0.5000	0.3304			
307.85	0.5000	0.4376			
314.05	0.5000	0.5274			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Eastman Kodak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

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	0.1233
0.1733	0.1466	0.1538
0.2982	0.2432	0.1843
0.4731	0.3658	0.2268
0.6378	0.4662	0.2691
0.8319	0.5738	0.3103
1.0000	0.6579	0.3421

[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 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.

(3) 99.8+ %, Spectroanalyzed, Fisher Scienitific, Pittsburgh, Pennsylvania, USA.

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) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

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	0.1381
0.1369	0.1151	0.1594
0.3185	0.2568	0.1938
0.5046	0.3865	0.2340
0.7099	0.5101	0.2815
0.8131	0.5650	0.3051
1.0000	0.6579	0.3421

[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 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.

(3) 99.8+ %, Spectroanalyzed, Fisher Scientific.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.3421
0.1654	0.1123	0.3213
0.3387	0.2367	0.3015
0.5215	0.3786	0.2740
0.6833	0.5143	0.2474
0.8507	0.6649	0.2184
1.0000	0.8079	0.1921

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) 99.8+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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.

Choi, P.B.; McLauglin, E.
Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.95	0.0000	0.4833	329.1	0.3000	0.7816
313.85	0.0000	0.5561	335.1	0.3000	0.8626
316.85	0.0000	0.5932			
323.65	0.0000	0.6897	295.9	1.0000	0.3851
328.95	0.0000	0.7711	298.4	1.0000	0.4071
333.15	0.0000	0.8422	309.7	1.0000	0.5218
			317.0	1.0000	0.6060
304.2	0.3000	0.4483	329.5	1.0000	0.7653
308.7	0.3000	0.5117	334.8	1.0000	0.8698
317.1	0.3000	0.6033			
323.5	0.3000	0.6882			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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.

Choi, P.B.; McLaughlin, E.
Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
302.35	0.0000	0.2348	331.5	0.3000	0.8006
310.45	0.0000	0.3540	337.4	0.3000	0.9109
314.65	0.0000	0.4319			
320.85	0.0000	0.5616	295.9	1.0000	0.3851
326.95	0.0000	0.6929	298.4	1.0000	0.4071
333.05	0.0000	0.8252	309.7	1.0000	0.5218
			317.0	1.0000	0.6060
306.8	0.3000	0.3785	329.5	1.0000	0.7653
314.7	0.3000	0.5221	334.8	1.0000	0.8698
320.4	0.3000	0.6150			
327.2	0.3000	0.7137			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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.

Choi, P.B.; McLaughlin, E.
Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.95	0.0000	0.4833	333.6	0.3000	0.8270
313.85	0.0000	0.5561	336.8	0.3000	0.8797
316.85	0.0000	0.5932			
323.65	0.0000	0.6897	297.3	1.0000	0.3742
328.95	0.0000	0.7711	300.9	1.0000	0.4085
333.15	0.0000	0.8422	307.1	1.0000	0.4743
			312.4	1.0000	0.5327
308.4	0.3000	0.4419	323.7	1.0000	0.6884
314.7	0.3000	0.5184	331.7	1.0000	0.8170
321.2	0.3000	0.6289			
326.9	0.3000	0.7287			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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.

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Choi, P.B.
Ph.D. Dissertation, LSU, USA (1982).

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
302.35	0.0000	0.2348	334.5	0.3000	0.8583
310.45	0.0000	0.3540	336.4	0.3000	0.8948
314.65	0.0000	0.4319			
320.85	0.0000	0.5616	297.3	1.0000	0.3742
326.95	0.0000	0.6929	300.9	1.0000	0.4085
333.05	0.0000	0.8252	307.1	1.0000	0.4743
			312.4	1.0000	0.5327
312.4	0.3000	0.5029	323.7	1.0000	0.6884
317.6	0.3000	0.5744	331.7	1.0000	0.8170
322.1	0.3000	0.6475			
326.3	0.3000	0.7168			
332.4	0.3000	0.8232			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

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

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, J.
J. Solution Chem. 1988, *16*, 519-534.

Choi, P.B.; McLaughlin, J.
Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
297.3	0.0000	0.3742	331.4	0.7000	0.8061
300.9	0.0000	0.4085	334.3	0.7000	0.8512
307.1	0.0000	0.4743			
312.4	0.0000	0.5327	295.9	1.0000	0.3851
323.7	0.0000	0.6884	298.4	1.0000	0.4071
331.7	0.0000	0.8170	309.7	1.0000	0.5218
			317.0	1.0000	0.6060
304.9	0.7000	0.4483	329.5	1.0000	0.7653
308.3	0.7000	0.4990	334.8	1.0000	0.8698
317.6	0.7000	0.6046			
324.2	0.7000	0.6957			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
305.6	0.0000	0.4528	328.7	0.5000	0.7487
310.5	0.0000	0.5060	334.2	0.5000	0.8509
314.6	0.0000	0.5556			
319.2	0.0000	0.6185	309.0	1.0000	0.3611
322.7	0.0000	0.6708	316.0	1.0000	0.4740
326.9	0.0000	0.7339	318.2	1.0000	0.5180
			324.3	1.0000	0.6406
302.7	0.5000	0.3665	328.2	1.0000	0.7385
310.1	0.5000	0.4599			
316.9	0.5000	0.5537			
323.5	0.5000	0.6563			

[a] $x_3^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over activated alumina and then recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

CARBAZOLE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

n-hexane + cyclohexane
n-heptane + cyclohexane
n-octane + cyclohexane
methylcyclohexane + cyclohexane
2,2,4-trimethylpentane + cyclohexane
cyclohexane + cyclooctane

II. Alkane + Aromatic Hydrocarbon

cyclohexane + benzene

III. Alkane + Ester

2,2,4-trimethylpentane + butyl butyrate

IV. Alkane + Ether

n-hexane + 1,1-oxybisbutane
n-heptane + 1,1-oxybisbutane
n-octane + 1,1-oxybisbutane
n-hexadecane + 1,1-oxybisbutane
cyclohexane + 1,1-oxybisbutane
cyclooctane + 1,1-oxybisbutane
methylcyclohexane + 1,1-oxybisbutane
2,2,4-trimethylpentane + 1,1-oxybisbutane
squalane + 1,1-oxybisbutane
t-butylcyclohexane + 1,1-oxybisbutane
2,2,4-trimethylpentane + 1,1-oxybispentane
n-hexane + tetrahydropyran
n-heptane + tetrahydropyran
n-hexadecane + tetrahydropyran
cyclohexane + tetrahydropyran
2,2,4-trimethylpentane + tetrahydropyran
t-butylcyclohexane + tetrahydropyran

V. Alkane + Chloroalkane

2,2,4-trimethylpentane + trichloromethane

VI. Ether + Chloroalkane

1,1-oxybisbutane + 1-chlorohexane
1,1-oxybisbutane + 1-chlorooctane
1,1-oxybisbutane + 1-chlorotetradecane
1,1-oxybisbutane + chlorocyclohexane

VII. Miscellaneous

2,2,4-trimethylpentane + 1-butanol
2,2,4-trimethylpentane + 1-octanol
benzene + trichloromethane
benzene + tetrachloromethane
methylbenzene + tetrachloromethane

CARBAZOLE SOLUBILITIES (Continued)

1,4-dimethylbenzene + tetrachloromethane
methylbenzene + pyridine
2-propanone + pyridine
2-propanone + methylbenzene
2-propanone + methanol
methanol + methylbenzene
ethanol + methylbenzene
2-propanol + methylbenzene
methylbenzene + phenol
2-propanone + carbon disulfide

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Phys. Chem. Liq. 1990, *22*, 157-162.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000139
0.1316	0.1316	0.000147
0.2887	0.2887	0.000154
0.3942	0.3941	0.000161
0.4631	0.4630	0.000165
0.6030	0.6029	0.000171
0.7289	0.7288	0.000176
0.8724	0.8722	0.000181
1.0000	0.9998	0.000183

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) 99 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Phys. Chem. Liq. 1990, *22*, 157-162.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000173
0.1538	0.1538	0.000178
0.2877	0.2877	0.000180
0.4165	0.4164	0.000182
0.5381	0.5380	0.000185
0.6574	0.6573	0.000186
0.7619	0.7618	0.000184
0.8738	0.8737	0.000184
1.0000	0.9998	0.000183

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) HPLC Grade, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Phys. Chem. Liq. 1990, *22*, 157-162.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000198
0.1449	0.1449	0.000200
0.2861	0.2860	0.000201
0.4315	0.4315	0.000198
0.5637	0.5636	0.000194
0.6890	0.6889	0.000192
0.7732	0.7731	0.000190
0.8826	0.8824	0.000187
1.0000	0.9998	0.000183

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(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.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Phys. Chem. Liq. 1990, *22*, 157-162.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000196
0.1463	0.1463	0.000195
0.2738	0.2737	0.000193
0.4366	0.4365	0.000191
0.5744	0.5743	0.000189
0.6903	0.6902	0.000188
0.7639	0.7638	0.000187
0.8576	0.8575	0.000185
1.0000	0.9998	0.000183

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(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.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Phys. Chem. Liq. 1990, *22*, 157-162.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000126
0.1478	0.1478	0.000133
0.2743	0.2743	0.000140
0.3768	0.3767	0.000145
0.5069	0.5068	0.000152
0.6029	0.6029	0.000158
0.7065	0.7064	0.000164
0.8537	0.8537	0.000173
1.0000	0.9998	0.000183

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(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.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Phys. Chem. Liq. 1990, *22*, 157-162.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000309
0.1715	0.1715	0.000289
0.2948	0.2947	0.000274
0.4369	0.4368	0.000256
0.5671	0.5670	0.000241
0.6839	0.6837	0.000226
0.7605	0.7603	0.000213
0.8760	0.8758	0.000198
1.0000	0.9998	0.000183

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_{10}N$; [86-74-8] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Benzene; C_6H_6; [71-43-2]	Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* 1967, *32*, 931-943.
VARIABLES:	**PREPARED BY:**
T/K = 293 and 298 Solvent Composition	W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C			t = 25 °C		
$x_3^{(s),b}$	x_3	x_1	$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.000153	0.000	0.000	0.000224
0.350	0.350	0.000672	0.350	0.350	0.000940
0.519	0.518	0.00119	0.519	0.518	0.00142
0.683	0.682	0.00190	0.683	0.681	0.00231
1.000	0.997	0.00352	1.000	0.996	0.00412

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00077	0.4054	0.00307
0.00697	0.000853	0.8132	0.00633
0.00971	0.000882	0.9960	0.00778
0.02871	0.000932	1.5128	0.0133
0.06130	0.00105	2.0038	0.0194
0.07538	0.00121	2.9994	0.0354
0.10420	0.00134	3.7227	0.0493
0.1561	0.00162	5.0024	0.0786
0.2057	0.00188	5.9975	0.0994
0.2494	0.00205		
0.3001	0.00243		
0.3961	0.00309		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, was recrystallized from acetone-heptane.

(2) 99 %, Phillips Petroleum Bartlesville, Oklahoma, USA.

(3) Purity not specified, Eastman Chemical Chemical Company, Rochester, New York, USA, was shaken with sodium hydroxide solution, washed with distilled water, dried over anhydrous magnesium sulfate, and distilled.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1 (compiler).
$c_3^{(s)}$: 4 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000139
0.0789	0.0789	0.000333
0.1602	0.1601	0.000590
0.2498	0.2496	0.000838
0.3404	0.3400	0.001166
0.4368	0.4361	0.001615
0.5382	0.5371	0.002049
0.6435	0.6418	0.002662
0.7581	0.7555	0.003392
0.8748	0.8713	0.003963
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000173
0.0906	0.0906	0.000392
0.1816	0.1815	0.000642
0.2738	0.2735	0.000943
0.3632	0.3627	0.001301
0.4672	0.4664	0.001771
0.5620	0.5607	0.002275
0.6640	0.6622	0.002761
0.7654	0.7629	0.003263
0.8739	0.8704	0.004012
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000198
0.1028	0.1028	0.000474
0.2030	0.2028	0.000804
0.2963	0.2960	0.001120
0.3835	0.3829	0.001492
0.4902	0.4893	0.001864
0.5949	0.5934	0.002463
0.6907	0.6887	0.002966
0.7885	0.7857	0.003605
0.8873	0.8835	0.004339
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000414
0.1380	0.1379	0.000807
0.2098	0.2096	0.001020
0.3130	0.3126	0.001360
0.4032	0.4025	0.001680
0.4774	0.4764	0.002020
0.5818	0.5804	0.002370
0.7127	0.7105	0.003080
0.8009	0.7979	0.003710
0.9146	0.9107	0.004300
1.0000	0.9950	0.005011

[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 tetrachloromethane. 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 used as received.

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

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 2 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000183
0.0665	0.0665	0.000442
0.1372	0.1363	0.000687
0.2143	0.2141	0.001013
0.2975	0.2971	0.001434
0.3876	0.3869	0.001772
0.4895	0.4884	0.002296
0.5996	0.5979	0.002888
0.7135	0.7111	0.003406
0.8510	0.8475	0.004103
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000309
0.0859	0.0858	0.000747
0.1689	0.1687	0.001098
0.2523	0.2519	0.001511
0.3438	0.3431	0.002028
0.4423	0.4412	0.002520
0.5445	0.5429	0.002997
0.6486	0.6464	0.003431
0.7699	0.7667	0.004120
0.8629	0.8589	0.004578
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000196
0.0877	0.0877	0.000500
0.1650	0.1649	0.000797
0.2453	0.2450	0.001123
0.3347	0.3342	0.001545
0.4294	0.4286	0.001959
0.5339	0.5326	0.002450
0.6885	0.6862	0.003278
0.7417	0.7390	0.003656
0.8568	0.8531	0.004356
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000126
0.1026	0.1026	0.000350
0.1971	0.1970	0.000596
0.2948	0.2945	0.000901
0.3911	0.3906	0.001246
0.4933	0.4924	0.001761
0.5933	0.5919	0.002303
0.6925	0.6906	0.002751
0.7878	0.7852	0.003356
0.8888	0.8852	0.004081
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_{10}N$; [86-74-8] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 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, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00077	1.2024	0.00382
0.0109	0.000816	1.4978	0.00478
0.0299	0.000856	1.9977	0.00650
0.0495	0.000902	3.031	0.0109
0.0847	0.000966	3.983	0.0162
0.1246	0.00105	4.763	0.0209
0.1998	0.00119	5.867	0.0287
0.4216	0.00172		
0.6936	0.00233		
0.8675	0.00286		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, was recrystallized from acetone-heptane.

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

(3) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1 (compiler).
$c_3^{(s)}$: 4 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2,6,10,15,19,23-Hexamethyltetracosane; $C_{30}H_{62}$; [111-01-3]

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000671
0.1604	0.1602	0.001070
0.1664	0.1662	0.001081
0.2687	0.2683	0.001320
0.4471	0.4463	0.001849
0.5693	0.5680	0.002340
0.5757	0.5743	0.002411
0.6726	0.6708	0.002740
0.7784	0.7759	0.003209
0.8289	0.8260	0.003558
0.9030	0.8992	0.004130
0.9625	0.9578	0.004701
1.0000	0.9950	0.005011

[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 tetrachloromethane. 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 Comapny, was used as received.

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

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 2 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Solution Chem. 1988, *17*, 1081-1091.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W.
J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000250
0.1123	0.1122	0.000643
0.2103	0.2100	0.001010
0.3018	0.3014	0.001416
0.4027	0.4019	0.001915
0.5065	0.5053	0.002323
0.6084	0.6067	0.002825
0.6435	0.6416	0.002972
0.7975	0.7944	0.003946
0.8989	0.8949	0.004405
1.0000	0.9950	0.005011

[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 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.

(3) Gold Label, 99+ %, 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) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00077	0.9446	0.00276
0.0186	0.000899	1.455	0.00415
0.0405	0.000956	1.938	0.00524
0.0590	0.000972	2.866	0.00881
0.0910	0.00105	4.002	0.0132
0.1201	0.00106	4.923	0.0182
0.2068	0.00124		
0.3993	0.00158		
0.5860	0.00195		
0.7813	0.00233		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, was recrystallized from acetone-heptane.

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

(3) Purity not specified, 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 shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1 (compiler).
$c_3^{(s)}$: 3 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000139
0.1442	0.1439	0.002243
0.2555	0.2542	0.005188
0.3674	0.3642	0.008676
0.4701	0.4642	0.01259
0.5741	0.5640	0.01761
0.6684	0.6533	0.02257
0.8405	0.8138	0.03180
0.9262	0.8913	0.03763
1.0000	0.9572	0.04284

[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 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.

(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: ± 2-4 % (relative error; 2 % for smaller x_1; 4 % for larger x_1.)

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000173
0.0480	0.0480	0.000496
0.1188	0.1187	0.001142
0.2475	0.2468	0.002993
0.3656	0.3637	0.005155
0.5020	0.4973	0.009344
0.5988	0.5905	0.01381
0.7161	0.7012	0.02081
0.8172	0.7941	0.02821
0.9119	0.8790	0.03608
1.0000	0.9572	0.04284

[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 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.

(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: ± 2-4 % (relative error; 2 % for smaller x_1; 4 % for larger x_1).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000414
0.0745	0.0744	0.000985
0.1539	0.1536	0.001723
0.2686	0.2678	0.003019
0.3531	0.3516	0.004235
0.4315	0.4291	0.005579
0.5332	0.5289	0.007994
0.6396	0.6318	0.01215
0.7495	0.7359	0.01812
0.8487	0.8277	0.02473
0.9411	0.9087	0.03439
1.0000	0.9572	0.04284

[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 tetrachloromethane. 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 used as received.

(3) 99 %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 2-4 % (relative error; 2 % for smaller x_1; and 4 % for larger x_1).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000183
0.1192	0.1190	0.001509
0.2183	0.2176	0.003271
0.3270	0.3250	0.006033
0.3861	0.3831	0.007828
0.5230	0.5161	0.01325
0.6259	0.6144	0.01832
0.7204	0.7035	0.02339
0.8172	0.7920	0.03082
0.9079	0.8738	0.03761
1.0000	0.9572	0.04284

[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 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 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: ± 2-4 % (relative error; 2 % for smaller x_1; 4 % for larger x_1).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000126
0.1394	0.1393	0.001041
0.2076	0.2073	0.001652
0.3032	0.3023	0.002863
0.3949	0.3931	0.004538
0.5021	0.4984	0.007441
0.6073	0.6004	0.01138
0.6992	0.6880	0.01602
0.8007	0.7823	0.02297
0.9032	0.8742	0.03210
1.0000	0.9572	0.04284

[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 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.

(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: ± 2-4 % (relative error; 2 % for smaller x_1; 4 % for larger x_1).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000250
0.0889	0.0888	0.001087
0.1997	0.1992	0.002499
0.3093	0.3079	0.004449
0.4025	0.3998	0.006748
0.4873	0.4829	0.009092
0.6116	0.6029	0.01419
0.7072	0.6931	0.01992
0.8036	0.7831	0.02549
0.9041	0.8737	0.03361
1.0000	0.9572	0.04284

[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 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.

(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: ± 2-4 % (relative error; 2 % for smaller x_1; 4 % for larger x_1).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00077	0.7838	0.00130
0.01030	0.000762	0.9948	0.00141
0.02132	0.000783	1.4740	0.00187
0.04185	0.000780	1.9654	0.00244
0.0698	0.000799	2.5007	0.00324
0.0996	0.000815	2.9785	0.00395
0.1548	0.000842	4.0055	0.00582
0.2037	0.000859	5.9623	0.0115
0.2523	0.000898	8.3823	0.0214
0.3014	0.000918	10.2973	0.0337
0.3949	0.000933	12.396	0.0468
0.5023	0.00126		
0.5904	0.00118		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, was recrystallized from acetone-heptane.

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

(3) Purity not specified, Fisher Scientific, Pittsburgh, Pennsylvania, USA, washed with distilled water, stored over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1 (compiler).
$c_3^{(s)}$: 4 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1] (3) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5]	Acree, W.E., Jr.; McCargar, J.W. *J. Pharm. Sci.* 1987, *76*, 575-579.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00255
0.0853	0.0850	0.00335
0.1727	0.1720	0.00396
0.2722	0.2709	0.00461
0.3475	0.3457	0.00509
0.4481	0.4458	0.00510
0.5491	0.5462	0.00526
0.6531	0.6496	0.00533
0.7594	0.7554	0.00532
0.8725	0.8679	0.00530
1.0000	0.9950	0.00501

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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.

(3) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00242
0.1102	0.1099	0.00317
0.2004	0.1996	0.00385
0.3017	0.3004	0.00438
0.3994	0.3975	0.00479
0.5056	0.5030	0.00518
0.6027	0.5995	0.00532
0.6938	0.6901	0.00536
0.7907	0.7865	0.00537
0.8950	0.8903	0.00527
1.0000	0.9950	0.00501

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Comapny, 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.

(3) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1] (3) 1-Chlorotetradecane; $C_{14}H_{29}Cl$; [2425-54-9]	McCargar, J.W.; Acree, W.E., Jr. *J. Solution Chem.* 1989, *18*, 151-158.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00240
0.1296	0.1292	0.00306
0.2272	0.2264	0.00356
0.3220	0.3207	0.00418
0.4069	0.4050	0.00457
0.5140	0.5115	0.00486
0.6135	0.6103	0.00523
0.7079	0.7043	0.00512
0.8072	0.8031	0.00513
0.8973	0.8928	0.00505
1.0000	0.9950	0.00501

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 tetrachloromethane. 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.

(3) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and J.W. McCargar

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00291
0.0799	0.0796	0.00385
0.1903	0.1894	0.00489
0.2947	0.2931	0.00543
0.4116	0.4091	0.00596
0.5138	0.5108	0.00591
0.6156	0.6119	0.00598
0.7023	0.6982	0.00585
0.7935	0.7890	0.00571
0.8895	0.8847	0.00538
1.0000	0.9950	0.00501

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 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 before use.

(3) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]
t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00077	0.6219	0.00342
0.00606	0.000767	0.8034	0.00442
0.00902	0.000781	1.0010	0.00543
0.01868	0.000808	1.0031	0.00542
0.03030	0.000845	1.5196	0.00831
0.04519	0.000939	1.9594	0.0104
0.07571	0.00110	3.0962	0.0162
0.1119	0.00128	4.0244	0.0205
0.1564	0.00146	6.0554	0.0297
0.2031	0.00166	8.0068	0.0375
0.3031	0.00210	10.874	0.0493
0.3958	0.00262		
0.3990	0.00267		
0.6001	0.00366		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, was recrystallized from acetone-heptane.

(2) 99 %, Phillips Petroleum Bartlesville, Oklahoma, USA.

(3) puriss, 99.5 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1 (compiler).
$c_3^{(s)}$: to 4 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$c_3^{(s)}$	c_1	$c_3^{(s)}$	c_1
0.00000	0.00077	0.03897	0.000992
0.00524	0.000792	0.05931	0.00111
0.01020	0.000828	0.08065	0.00123
0.01085	0.000786	0.1226	0.00153
0.01206	0.000810	0.2120	0.00209
0.01360	0.000812	0.4360	0.00336
0.01425	0.000840	0.6914	0.00490
0.01517	0.000839	0.7780	0.00587
0.01635	0.000840	1.033	0.00704
0.01762	0.000822	1.970	0.0145
0.01847	0.000874	2.958	0.0225
0.02070	0.000894	3.941	0.0315
0.02248	0.000857	4.997	0.0404
0.02516	0.000874	6.313	0.0515
0.02778	0.00101		

[a] $c_3^{(s)}$: initial molar concentration (mol dm^{-3}) of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass vials, and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several duplicate 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, was recrystallized from acetone-heptane.

(2) 99 %, Phillips Petroleum Bartlesville, Oklahoma, USA.

(3) 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1 (compiler).
$c_3^{(s)}$: 4 sig. figs. (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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 = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00478
0.246	0.245	0.00411
0.396	0.394	0.00396
0.567	0.565	0.00398
1.000	0.995	0.00412

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00352
0.145	0.145	0.00327
0.203	0.202	0.00278
0.336	0.335	0.00257
0.504	0.503	0.00203
1.000	0.999	0.000659

t = 25 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00412
0.203	0.202	0.00328
0.337	0.336	0.00286
0.504	0.503	0.00242
1.000	0.999	0.000899

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00374
0.166	0.166	0.00293
0.375	0.374	0.00232
0.473	0.472	0.00205
0.642	0.641	0.00152
0.844	0.843	0.00107
1.000	0.999	0.000659

t = 40 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00666
0.083	0.083	0.00590
0.166	0.165	0.00530
0.375	0.373	0.00418
0.473	0.471	0.00393
0.642	0.640	0.00292
0.844	0.842	0.00213
1.000	0.998	0.00165

t = 60 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.0111
0.084	0.083	0.0102
0.166	0.164	0.00941
0.375	0.372	0.00800
0.642	0.638	0.00585
0.844	0.840	0.00445
1.000	0.996	0.00377

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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 = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00483
0.256	0.255	0.00396
0.408	0.407	0.00315
0.580	0.579	0.00242
1.000	0.999	0.000772

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.

x_2: ± 0.001 (compiler).

x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 20.0$ °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00375
0.057	0.057	0.00737
0.077	0.076	0.00854
0.114	0.113	0.0120
0.170	0.167	0.0167
0.226	0.221	0.0208
0.280	0.272	0.0290
0.538	0.510	0.0513
0.777	0.722	0.0713
1.000	0.910	0.0895

$t = 40$ °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00666
0.115	0.113	0.0163
0.280	0.269	0.0385
0.538	0.503	0.0648
0.778	0.708	0.0895
1.000	0.890	0.110

$t = 60$ °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.0111
0.115	0.112	0.0236
0.279	0.265	0.0516
0.538	0.494	0.0824
0.777	0.690	0.112
1.000	0.862	0.138

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) 2-Propanone; C_3H_6O; [67-64-1]

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.0924
0.313	0.290	0.0732
0.576	0.545	0.0545
0.803	0.772	0.0391
1.000	0.976	0.0239

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) 2-Propanone; C_3H_6O; [67-64-1]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

$T/K = 293$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 20.0\ ^{\circ}C$

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00374
0.148	0.147	0.00925
0.346	0.340	0.0160
0.613	0.599	0.0235
0.826	0.805	0.0258
0.934	0.910	0.0254
1.000	0.976	0.0239

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]
t = 20.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00183
0.057	0.057	0.00256
0.221	0.220	0.00382
0.269	0.267	0.00704
0.453	0.448	0.0120
0.688	0.675	0.0189
0.832	0.814	0.0216
1.000	0.976	0.0239

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00183
0.033	0.033	0.00227
0.104	0.104	0.00319
0.258	0.257	0.00483
0.510	0.507	0.00660
0.582	0.578	0.00689
0.759	0.754	0.00648
0.868	0.863	0.00574
1.000	0.996	0.00374

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

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

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00332
0.052	0.052	0.00407
0.133	0.132	0.00521
0.332	0.330	0.00660
0.429	0.426	0.00719
0.600	0.595	0.00769
0.818	0.813	0.00647
1.000	0.996	0.00374

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) 2-Propanol; C_3H_8O; [67-63-0]

(3) 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
Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00277
0.067	0.067	0.00374
0.179	0.178	0.00552
0.395	0.392	0.00795
0.495	0.491	0.00809
0.662	0.657	0.00762
1.000	0.996	0.00374

t = 40 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00523
0.179	0.177	0.00902
0.302	0.299	0.0107
0.395	0.390	0.0123
0.495	0.489	0.0129
0.662	0.653	0.0131
0.854	0.845	0.0106
1.000	0.993	0.00666

t = 60 °C

$x_3^{(s),b}$	x_3	x_1
0.000	0.000	0.00912
0.180	0.177	0.0148
0.219	0.215	0.0161
0.395	0.387	0.0195
0.662	0.649	0.0202
1.000	0.989	0.0111

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

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(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_3: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) 2-Propanone; C_3H_6O; [67-64-1]

(3) 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, Solvent Composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00149
0.304	0.296	0.0269
0.567	0.546	0.0367
0.686	0.661	0.0370
0.798	0.770	0.0345
1.000	0.976	0.0239

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the 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.

(3) 99 %, Commerical sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

DIBENZOFURAN SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

None

II. Alkane + Aromatic Hydrocarbon

None

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + pyridine
cyclohexane + pyridine
benzene + thiophene
cyclohexane + thiophene
thiophene + pyridine
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
321.9	0.0000	0.4797	323.7	1.0000	0.5083
323.5	0.0000	0.5068	326.2	1.0000	0.5446
329.4	0.0000	0.5844	331.2	1.0000	0.6161
332.0	0.0000	0.6222	336.3	1.0000	0.6812
338.7	0.0000	0.7224	340.8	1.0000	0.7582
312.3	0.3000	0.4004			
322.2	0.3000	0.5093			
329.2	0.3000	0.5951			
337.1	0.3000	0.7031			
343.4	0.3000	0.8079			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
327.8	0.0000	0.4226	323.7	1.0000	0.5083
330.2	0.0000	0.4805	326.2	1.0000	0.5446
334.0	0.0000	0.5436	331.2	1.0000	0.6161
337.5	0.0000	0.6300	336.3	1.0000	0.6812
338.5	0.0000	0.6700	340.8	1.0000	0.7582
345.1	0.0000	0.8120			
309.7	0.3000	0.3153			
318.0	0.3000	0.4027			
325.0	0.3000	0.4925			
331.8	0.3000	0.6060			
335.9	0.3000	0.6567			
346.7	0.3000	0.8465			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized from toluene.

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

(3) Gold Label, 99.9+ %, Aldrich Chemical Company was used

ESTIMATED ERRORS:

T/K: ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
321.9	0.0000	0.4797	314.2	1.0000	0.4220
323.5	0.0000	0.5068	319.2	1.0000	0.4757
329.4	0.0000	0.5844	322.3	1.0000	0.5083
332.0	0.0000	0.6222	332.8	1.0000	0.6347
338.7	0.0000	0.7224	337.0	1.0000	0.6960
			341.1	1.0000	0.7585
303.3	0.3000	0.3069			
312.7	0.3000	0.3919			
324.2	0.3000	0.5179			
329.6	0.3000	0.5910			
339.8	0.3000	0.7356			
344.5	0.3000	0.8130			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
327.8	0.0000	0.4226	314.2	1.0000	0.4220
330.2	0.0000	0.4805	319.3	1.0000	0.4757
334.0	0.0000	0.5436	322.3	1.0000	0.5083
337.5	0.0000	0.6300	332.8	1.0000	0.6347
338.5	0.0000	0.6700	337.0	1.0000	0.6960
345.1	0.0000	0.8120	341.1	1.0000	0.7585
318.4	0.3000	0.3633			
326.4	0.3000	0.4837			
329.6	0.3000	0.5402			
334.0	0.3000	0.6170			
341.2	0.3000	0.7436			
347.4	0.3000	0.8629			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
314.2	0.0000	0.4220	338.0	0.3000	0.7151
319.3	0.0000	0.4757	344.0	0.3000	0.8111
322.3	0.0000	0.5083			
332.8	0.0000	0.6347	323.7	1.0000	0.5083
337.0	0.0000	0.6960	326.2	1.0000	0.5446
341.1	0.0000	0.7585	331.2	1.0000	0.6161
			336.3	1.0000	0.6812
299.9	0.3000	0.2758	340.8	1.0000	0.7582
312.6	0.3000	0.4083			
321.1	0.3000	0.4925			
329.9	0.3000	0.6073			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
318.9	0.0000	0.4521	328.6	0.5000	0.5496
322.6	0.0000	0.4907	343.5	0.5000	0.7999
326.6	0.0000	0.5494			
337.9	0.0000	0.6990	326.4	1.0000	0.4245
339.5	0.0000	0.7330	328.2	1.0000	0.4646
			331.5	1.0000	0.5110
308.7	0.5000	0.1693	333.5	1.0000	0.5752
317.5	0.5000	0.2412	337.2	1.0000	0.6447
325.7	0.5000	0.3278			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Comapny, Milwaukee, Wisconsin, USA, was recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

$x_3^{(s)}$: ± 0.0001.

x_1: ± 0.0003.

DIBENZOTHIOPHENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

None

II. Alkane + Aromatic Hydrocarbon

None

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + pyridine
cyclohexane + pyridine
benzene + thiophene
cyclohexane + thiophene
thiophene + pyridine
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
309.9	0.0000	0.1896	306.5	1.0000	0.2143
315.3	0.0000	0.2246	313.0	1.0000	0.2552
327.8	0.0000	0.3347	322.8	1.0000	0.3313
337.2	0.0000	0.4362	327.4	1.0000	0.3784
342.3	0.0000	0.5144	334.7	1.0000	0.4498
			335.2	1.0000	0.4652
308.8	0.3000	0.2060			
319.8	0.3000	0.2856			
332.0	0.3000	0.4012			
340.6	0.3000	0.5024			
348.0	0.3000	0.5964			
355.9	0.3000	0.7237			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
320.6	0.0000	0.0871	352.0	0.3000	0.6329
326.6	0.0000	0.1129	357.7	0.3000	0.7336
328.2	0.0000	0.1294			
335.8	0.0000	0.1999	306.5	1.0000	0.2143
343.0	0.0000	0.3154	313.0	1.0000	0.2552
343.3	0.0000	0.3346	322.8	1.0000	0.3313
			327.4	1.0000	0.3784
319.8	0.3000	0.2141	334.7	1.0000	0.4498
330.5	0.3000	0.3174	335.2	1.0000	0.4652
339.2	0.3000	0.4231			
345.0	0.3000	0.5150			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
309.9	0.0000	0.1896	349.1	0.3000	0.6080
315.3	0.0000	0.2246	355.4	0.3000	0.7103
327.8	0.0000	0.3347			
337.2	0.0000	0.4362	309.3	1.0000	0.2379
342.3	0.0000	0.5144	315.2	1.0000	0.2776
			322.7	1.0000	0.3361
308.7	0.3000	0.2008	327.0	1.0000	0.3743
323.2	0.3000	0.3100	328.1	1.0000	0.3872
333.1	0.3000	0.4051	337.0	1.0000	0.4950
341.0	0.3000	0.5025			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
320.6	0.0000	0.0871	348.5	0.3000	0.5381
326.6	0.0000	0.1129	355.1	0.3000	0.6704
328.2	0.0000	0.1294			
335.8	0.0000	0.1999	309.3	1.0000	0.2379
343.0	0.0000	0.3154	315.2	1.0000	0.2776
343.3	0.0000	0.3346	322.7	1.0000	0.3361
			327.0	1.0000	0.3743
322.3	0.3000	0.1617	328.1	1.0000	0.3872
333.6	0.3000	0.2737	337.0	1.0000	0.4950
339.3	0.3000	0.3647			
345.8	0.3000	0.4805			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
309.3	0.0000	0.2379	345.8	0.3000	0.5871
315.2	0.0000	0.2776	353.1	0.3000	0.7012
322.7	0.0000	0.3361			
327.0	0.0000	0.3743	306.5	1.0000	0.2143
328.1	0.0000	0.3872	313.0	1.0000	0.2552
337.0	0.0000	0.4950	322.8	1.0000	0.3313
			327.4	1.0000	0.3784
304.9	0.3000	0.2096	334.7	1.0000	0.4498
316.8	0.3000	0.2906	335.2	1.0000	0.4652
329.5	0.3000	0.3994			
339.0	0.3000	0.5071			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
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]

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
308.7	0.0000	0.2163	343.1	0.5000	0.5102
318.2	0.0000	0.2781	349.2	0.5000	0.6089
326.6	0.0000	0.3508			
336.3	0.0000	0.4466	311.3	1.0000	0.1056
337.8	0.0000	0.4692	318.9	1.0000	0.1393
			325.8	1.0000	0.1859
303.7	0.5000	0.1402	333.9	1.0000	0.2628
314.3	0.5000	0.1964			
327.6	0.5000	0.3077			
337.0	0.5000	0.4194			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

FLUORANTHENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

None

II. Alkane + Aromatic Hydrocarbon

None

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

methylbenzene + 2-propanone
methylbenzene + ethanol
methylbenzene + pyridine

COMPONENTS:

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

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

(3) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s)}$,b	x_2	x_1
0.000	0.000	0.0711
0.150	0.124	0.0911
0.296	0.264	0.109
0.387	0.342	0.116
0.486	0.428	0.120
0.715	0.628	0.122
1.000	0.895	0.105

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

(3) Commerical sample, purity and source not specified, was dehydrated and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.

x_2: ± 0.001 (compiler).

x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00514
0.111	0.110	0.0102
0.250	0.245	0.0209
0.429	0.411	0.0411
0.666	0.619	0.0711
0.818	0.744	0.0905
1.000	0.895	0.105

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

(3) Commercial sample, purity and source not specified, was dehydrated and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.158
0.177	0.149	0.156
0.364	0.309	0.151
0.562	0.482	0.143
0.775	0.676	0.128
1.000	0.895	0.105

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

(3) Purity not specified, Urxovy Zavody, was treated with potassium permanganate, dried over potassium hydroxide and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

FLUORENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

None

II. Alkane + Aromatic Hydrocarbon

cyclohexane + benzene

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + pyridine
cyclohexane + pyridine
benzene + thiophene
cyclohexane + thiophene
thiophene + pyridine
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
310.95	0.0000	0.0537	351.45	0.5000	0.4636
316.25	0.0000	0.0684	359.35	0.5000	0.5730
321.75	0.0000	0.0871			
327.35	0.0000	0.1122	311.65	0.7000	0.1596
331.85	0.0000	0.1384	330.35	0.7000	0.2777
336.45	0.0000	0.1733	339.85	0.7000	0.3603
341.45	0.0000	0.2200	346.85	0.7000	0.4353
346.25	0.0000	0.2787	356.55	0.7000	0.5477
319.65	0.3000	0.1346	307.75	1.0000	0.1665
327.45	0.3000	0.1809	313.45	1.0000	0.1950
342.15	0.3000	0.3111	318.15	1.0000	0.2215
350.65	0.3000	0.4192	323.05	1.0000	0.2528
359.25	0.3000	0.5471	330.45	1.0000	0.3055
			336.25	1.0000	0.3525
317.05	0.5000	0.1558	340.65	1.0000	0.3957
331.95	0.5000	0.2548	348.35	1.0000	0.4744
343.15	0.5000	0.3643	354.85	1.0000	0.5477

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 97.9 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, 22, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.75	0.0000	0.1665	333.1	0.3000	0.3394
313.45	0.0000	0.1950	351.6	0.3000	0.5031
318.15	0.0000	0.2215	359.8	0.3000	0.6042
323.05	0.0000	0.2528			
330.45	0.0000	0.3055	311.5	1.0000	0.1979
336.25	0.0000	0.3525	327.1	1.0000	0.2936
340.65	0.0000	0.3957	340.2	1.0000	0.4002
348.35	0.0000	0.4744	349.0	1.0000	0.4909
354.85	0.0000	0.5477	359.2	1.0000	0.6127
308.7	0.3000	0.1845			
326.0	0.3000	0.2736			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
310.95	0.0000	0.0537	343.0	0.3000	0.3898
316.25	0.0000	0.0684	347.1	0.3000	0.4314
321.75	0.0000	0.0871			
327.35	0.0000	0.1122	311.5	1.0000	0.1979
331.85	0.0000	0.1384	327.1	1.0000	0.2936
336.45	0.0000	0.1733	340.2	1.0000	0.4002
341.45	0.0000	0.2200	349.0	1.0000	0.4909
346.25	0.0000	0.2787	359.2	1.0000	0.6127
325.8	0.3000	0.2261			
333.4	0.3000	0.2836			
335.8	0.3000	0.3088			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.75	0.0000	0.1665	331.9	0.3000	0.3332
313.45	0.0000	0.1950	339.3	0.3000	0.3959
318.15	0.0000	0.2215	347.5	0.3000	0.4793
323.05	0.0000	0.2528	354.0	0.3000	0.5530
330.45	0.0000	0.3055			
336.25	0.0000	0.3525	303.6	1.0000	0.1844
340.65	0.0000	0.3957	321.0	1.0000	0.2762
348.35	0.0000	0.4744	335.5	1.0000	0.3802
354.85	0.0000	0.5477	350.2	1.0000	0.5146
			357.5	1.0000	0.5954
303.0	0.3000	0.1578			
310.7	0.3000	0.1940			
317.4	0.3000	0.2316			
325.4	0.3000	0.2839			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
310.95	0.0000	0.0537	338.7	0.3000	0.3073
316.25	0.0000	0.0684	345.2	0.3000	0.3824
321.75	0.0000	0.0871	354.0	0.3000	0.5005
327.35	0.0000	0.1122			
331.85	0.0000	0.1384	303.6	1.0000	0.1844
336.45	0.0000	0.1733	321.0	1.0000	0.2762
341.45	0.0000	0.2200	335.5	1.0000	0.3802
346.25	0.0000	0.2787	350.2	1.0000	0.5146
			357.5	1.0000	0.5954
300.5	0.3000	0.0828			
308.6	0.3000	0.1108			
316.0	0.3000	0.1429			
322.7	0.3000	0.1792			
331.1	0.3000	0.2378			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
303.6	0.0000	0.1844	340.3	0.3000	0.4123
321.0	0.0000	0.2762	343.0	0.3000	0.4378
335.5	0.0000	0.3802			
350.2	0.0000	0.5146	311.5	1.0000	0.1979
357.5	0.0000	0.5954	327.1	1.0000	0.2936
			340.2	1.0000	0.4002
308.0	0.3000	0.1913	349.0	1.0000	0.4909
322.5	0.3000	0.2731	359.2	1.0000	0.6127
330.3	0.3000	0.3285			
335.2	0.3000	0.3644			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
303.6	0.0000	0.1672	357.2	0.5000	0.5568
311.7	0.0000	0.2075	364.2	0.5000	0.6565
322.8	0.0000	0.2695			
325.7	0.0000	0.2861	306.1	1.0000	0.0843
335.7	0.0000	0.3702	321.3	1.0000	0.1491
343.0	0.0000	0.4334	331.6	1.0000	0.2244
356.3	0.0000	0.5728	342.9	1.0000	0.3144
			353.0	1.0000	0.4445
309.7	0.5000	0.1515	366.2	1.0000	0.6671
327.0	0.5000	0.2540			
337.5	0.5000	0.3469			
347.0	0.5000	0.4493			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over activated alumina and then recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

NAPHTHALENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

n-hexane + cyclohexane
n-hexane + n-hexadecane
cyclohexane + n-hexadecane

II. Alkane + Aromatic Hydrocarbon

n-hexane + benzene
n-hexadecane + benzene
cyclohexane + benzene
n-hexane + methylbenzene
n-hexadecane + methylbenzene
cyclohexane + methylbenzene
n-hexane + ethylbenzene
n-hexadecane + ethylbenzene
cyclohexane + ethylbenzene

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

n-hexane + tetrachloromethane
n-hexadecane + tetrachloromethane
cyclohexane + tetrachloromethane

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + methylbenzene
benzene + tetrachloromethane
methylbenzene + ethylbenzene
methylbenzene + tetrachloromethane
ethylbenzene + tetrachloromethane
n-hexane + ethanol
n-hexane + 1-butanol
n-hexane + 1-hexanol
n-hexane + 1-octanol
benzene + pyridine
cyclohexane + pyridine
benzene + thiophene
cyclohexane + thiophene
thiophene + pyridine
benzene + ethylbenzene
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

NAPHTHALENE SOLUBILITIES (Continued)

cyclohexane + diiodomethane
trichloromethane + diethyl ether
carbon disulfide + diethyl ether
methanol + water
ethanol + water
1-propanol + water
1-butanol + water
1-pentanol + water
2-methyl-2-propanol + water
2-propanone + water
2-butanone + water
dimethyl sulfoxide + water
N,N-dimethylformamide + water
acetonitrile + water
1,2-ethanediol + water
urea + water

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *10*, 25-29.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2[b]	x_1
0.0000	0.0000	0.1487
0.1553	0.1327	0.1453
0.3996	0.3438	0.1396
0.6013	0.5220	0.1319
0.7986	0.6984	0.1255
1.0000	0.8832	0.1168

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by complier.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) Spectroquality, Matheson, Coleman and dried over phosphorous pentoxide and distilled to a final purity of 99.8 %.

ESTIMATED ERRORS:

T/K: ± 0.01.
$x_2^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *10*, 25-29.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2[b]	x_1
0.0000	0.0000	0.2043
0.1573	0.1270	0.1924
0.3964	0.3273	0.1743
0.5882	0.4943	0.1597
0.8511	0.7364	0.1348
1.0000	0.8832	0.1168

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) Practical Grade, Eastman Chemical Company, dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_2^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *10*, 25-29.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_2^{(s)}$	x_2[b]	x_1
0.0000	0.0000	0.2043
0.1689	0.1362	0.1935
0.4067	0.3341	0.1785
0.4181	0.3437	0.1779
0.5736	0.4772	0.1680
0.8289	0.7011	0.1542
1.0000	0.8513	0.1487

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.8 %.

(3) Practical Grade, Eastman Chemical Company, dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_2^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1168
0.0743	0.0645	0.1313
0.2121	0.1784	0.1590
0.4109	0.3276	0.2028
0.5960	0.4530	0.2400
0.8219	0.5964	0.2744
0.9506	0.6745	0.2905
1.0000	0.7054	0.2946

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.95 %.

(3) Spectroquality, Matheson, Coleman and Bell, dried over sodium and distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2043
0.1743	0.1381	0.2075
0.4219	0.3284	0.2217
0.6023	0.4593	0.2375
0.8603	0.6251	0.2734
1.0000	0.7054	0.2946

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester New York, USA, was used as received.

(2) Practical Grade, Eastman Chemical Company, dried over phosporous pentoxide and distilled to a final purity of 99.1 %.

(3) Spectroquality, Matheson, Coleman and Bell, dried over sodium and distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

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[b]	x_1
0.0000	0.0000	0.1487
0.0614	0.0514	0.1622
0.2045	0.1649	0.1935
0.4034	0.3104	0.2306
0.6006	0.4439	0.2609
0.7967	0.5722	0.2818
0.9411	0.6668	0.2915
1.0000	0.7054	0.2946

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, dried over phosphorous pentoxide and distilled to a final purity of 99.8 %.

(3) Spectroquality, Matheson, Coleman and Bell dried over sodium and distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
300.15	0.0000	0.1597	329.75	0.5000	0.6047
308.25	0.0000	0.2254	340.75	0.5000	0.7848
315.15	0.0000	0.3025			
325.45	0.0000	0.4612	299.65	0.7000	0.2844
333.15	0.0000	0.6073	312.65	0.7000	0.4045
343.05	0.0000	0.8082	321.55	0.7000	0.5071
			334.35	0.7000	0.6854
297.15	0.3000	0.2041	337.95	0.7000	0.7417
311.85	0.3000	0.3400			
323.55	0.3000	0.4931	310.35	1.0000	0.3964
326.05	0.3000	0.5308	315.55	1.0000	0.4494
339.25	0.3000	0.7535	323.45	1.0000	0.5391
			334.35	1.0000	0.6885
302.95	0.5000	0.2850	344.15	1.0000	0.8422
313.25	0.5000	0.3891			
318.65	0.5000	0.4520			
326.65	0.5000	0.5598			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.1.
$x_3^{(s)}$: $\pm$ 0.0001.
x_1: $\pm$ 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1168
0.2156	0.1807	0.1617
0.4076	0.3253	0.2018
0.5934	0.4518	0.2386
0.7910	0.5789	0.2681
1.0000	0.7080	0.2920

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) ACS Grade, Matheson, Coleman and Bell, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

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[b]	x_1
0.0000	0.0000	0.2043
0.1592	0.1260	0.2087
0.3968	0.3095	0.2199
0.5890	0.4505	0.2351
0.8399	0.6153	0.2674
1.0000	0.7080	0.2920

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Practical Grade, Eastman Chemical Comapny, was dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

(3) ACS Grade, Matheson, Coleman and Bell, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1487
0.2071	0.1668	0.1948
0.3733	0.2895	0.2246
0.5952	0.4426	0.2564
0.7928	0.5736	0.2765
1.0000	0.7080	0.2920

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, dried over phosphorous pentoxide and distilled to a final purity of 99.8 %.

(3) ACS Grade, Matheson, Coleman and Bell, dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1168
0.1663	0.1409	0.1526
0.4185	0.3322	0.2063
0.6053	0.4586	0.2423
0.8445	0.6118	0.2756
1.0000	0.7074	0.2926

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) ACS Grade, Matheson, Coleman and Bell, was dried over calcium hydride and distilled to a final purity of 99.9 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexadecane; $C_{16}H_{34}$; [544-76-3] (3) Ethylbenzene; C_8H_{10}; [100-41-4]	Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1965, *9*, 161-165.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2043
0.1874	0.1478	0.2113
0.4249	0.3287	0.2264
0.6190	0.4680	0.2440
0.8514	0.6196	0.2722
1.0000	0.7074	0.2926

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Practical Grade, Eastman Chemical Company dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

(3) ACS Grade, Matheson, Coleman and Bell dried over calcium hydride and distilled to a final purity of 99.9 %.

ESTIMATED ERRORS:

T/K: ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data <u>1965</u>, *9*, 161-165.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1487
0.1574	0.1284	0.1840
0.4135	0.3186	0.2295
0.6006	0.4484	0.2534
0.7930	0.5744	0.2757
1.0000	0.7074	0.2926

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) ACS Grade, Matheson, Coleman and Bell, was dried over calcium hydride and distilled to a final purity of 99.9 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *10*, 25-29.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1168
0.0221	0.0195	0.1191
0.2029	0.1742	0.1415
0.4315	0.3563	0.1742
0.5971	0.4790	0.1978
0.7997	0.6159	0.2298
0.9017	0.6811	0.2447
1.0000	0.7409	0.2591

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) Spectroquality, Matheson, Coleman and Bell dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexadecane; $C_{16}H_{34}$; [544-76-3] (3) Tetrachloromethane; CCl_4; [56-23-5]	Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1965, *10*, 25-29.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3^{b}	x_1
0.0000	0.0000	0.2043
0.1517	0.1213	0.2003
0.4057	0.3242	0.2009
0.5820	0.4622	0.2058
0.8410	0.6491	0.2282
1.0000	0.7409	0.2591

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Practical Grade, Eastman Chemical Company dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

(3) Spectroquality, Matheson, Coleman and Bell dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *10*, 25-29.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.1487
0.1939	0.1213	0.1723
0.3971	0.3242	0.1955
0.5883	0.4622	0.2169
0.7630	0.6491	0.2356
1.0000	0.7409	0.2591

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.8 %.

(3) Spectroquality, Matheson, Coleman and Bell, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Yeh, K.-N.

J. Chem. Eng. Data 1970, *15*, 13-17.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
292.95	0.0000	0.1345	288.16	0.3911	0.1317
301.83	0.0000	0.1720	292.88	0.3911	0.1587
306.71	0.0000	0.2122	304.09	0.3911	0.2420
318.28	0.0000	0.3463	315.68	0.3911	0.3658
326.75	0.0000	0.4849	321.00	0.3911	0.4384
334.01	0.0000	0.6244	329.55	0.3911	0.5719
340.06	0.0000	0.7455	333.62	0.3911	0.6420
346.75	0.0000	0.8762	343.16	0.3911	0.8137
292.22	0.1780	0.1318	287.86	0.5805	0.1439
306.07	0.1780	0.2318	302.38	0.5805	0.2500
313.35	0.1780	0.3093	309.63	0.5805	0.3182
318.80	0.1780	0.3797	319.79	0.5805	0.4417
325.86	0.1780	0.4899	327.41	0.5805	0.5505
332.96	0.1780	0.6154	337.29	0.5805	0.7125
339.41	0.1780	0.7386	342.95	0.5805	0.8122
342.94	0.1780	0.8057			

(Continued on next page)

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.50 rps while the bath temperature was slowly increased. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each composition.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, Baker Chemical Company, USA, was used as received.

(2) Reagent Grade, Baker Chemical Company.

(3) Reagent Grade, Baker Chemical Company.

Components 2 and 3 were stored over phosphorous pentoxide and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.03.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0001.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Yeh, K.-N.

J. Chem. Eng. Data 1970, *15*, 13-17.

VARIABLES:

Temperature and Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

T/K	$x_3^{(s)}$	x_1
285.24	0.7788	0.1530
297.22	0.7788	0.2293
308.67	0.7788	0.3296
318.24	0.7788	0.4384
327.44	0.7788	0.5635
335.65	0.7788	0.6928
342.20	0.7788	0.8022
286.64	1.0000	0.1812
290.51	1.0000	0.2039
300.17	1.0000	0.2738
316.25	1.0000	0.4329
323.84	1.0000	0.5269
328.58	1.0000	0.5915
334.92	1.0000	0.6880
342.33	1.0000	0.8065

[a] $x_3^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2920
0.3497	0.0645	0.2921
0.4014	0.1784	0.2908
0.6113	0.3276	0.2913
0.7759	0.4530	0.2931
0.9223	0.5964	0.2940
1.0000	0.7054	0.2946

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) ACS Grade, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) Spectroquality, Matheson, Coleman and Bell, was dried over sodium and distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2591
0.2880	0.2102	0.2702
0.3866	0.2813	0.2723
0.6634	0.4758	0.2828
0.8604	0.6105	0.2904
1.0000	0.7054	0.2946

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and and Bell dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

(3) Spectroquality, Matheson, Coleman and Bell dried over sodium and distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2926
0.1591	0.1126	0.2923
0.4117	0.2915	0.2919
0.6135	0.4346	0.2916
0.8332	0.5898	0.2921
1.0000	0.7080	0.2920

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over calcium hydride and distilled to a final purity of 99.9 %.

(3) ACS Grade, Matheson, Coleman and Bell, dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2591
0.2057	0.1509	0.2665
0.4129	0.2995	0.2747
0.5899	0.4247	0.2800
0.7942	0.5665	0.2867
1.0000	0.7080	0.2920

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) ACS Grade, Matheson, Coleman and Bell, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1965, *9*, 161-165.

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[b]	x_1
0.0000	0.0000	0.2591
0.1777	0.1309	0.2635
0.4095	0.2981	0.2720
0.6328	0.4558	0.2797
0.8408	0.5992	0.2873
1.0000	0.7074	0.2926

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

(3) ACS Grade, Matheson, Coleman and Bell, was dried over calcium hydride and distilled to a final purity of 99.9 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Domańska, U.

Polish J. Chem. 1981, *55*, 1715-1720.
(numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature and Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_2^{(s)}$	x_1	*T*/K	$x_2^{(s)}$	x_1
290.50	0.0000	0.024	279.70	0.5000	0.0435
294.30	0.0000	0.028	283.70	0.5000	0.0508
298.15	0.0000	0.032	287.60	0.5000	0.0598
302.20	0.0000	0.037	291.50	0.5000	0.0702
305.65	0.0000	0.042	294.80	0.5000	0.0806
308.80	0.0000	0.048	298.55	0.5000	0.0937
322.20	0.0000	0.087	302.35	0.5000	0.110
			307.15	0.5000	0.134
290.10	0.1769	0.0415	312.95	0.5000	0.173
292.90	0.1769	0.0465	316.25	0.5000	0.209
296.60	0.1769	0.0533	319.65	0.5000	0.250
300.20	0.1769	0.0617	323.45	0.5000	0.302
304.50	0.1769	0.0741	327.25	0.5000	0.376
307.55	0.1769	0.0878	331.70	0.5000	0.469
316.65	0.1769	0.130			
320.65	0.1769	0.159			

(Continued next page)

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Reachim, Poland, was dried over phosphorous pentoxide and fractionally distilled to a final purity of 99.9+ %.

(3) Initial purity not specified, Z.P. Spiryt. Lodz, was fractionally distilled to final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0002 (compiler).
x_1: to 3 significant figs. (compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexane; C_6H_{14}; [110-54-3] (3) Ethanol; C_2H_6O; [64-17-5]	Domańska, U. *Polish J. Chem.* 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)
VARIABLES: Temperature and Solvent Composition	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

T/K	$x_2^{(s)}$	x_1
280.75	0.6998	0.0534
284.80	0.6998	0.0629
294.35	0.6998	0.0924
299.15	0.6998	0.113
304.70	0.6998	0.136
308.35	0.6998	0.166
312.35	0.6998	0.201
317.05	0.6998	0.249
320.25	0.6998	0.293
323.40	0.6998	0.342
326.85	0.6998	0.402
334.00	0.6998	0.542
295.90	0.8584	0.107
300.30	0.8584	0.128
305.20	0.8584	0.158
310.60	0.8584	0.200
319.05	0.8584	0.294
282.05	1.0000	0.063
286.35	1.0000	0.072
289.55	1.0000	0.084
289.85	1.0000	0.082
292.45	1.0000	0.094
295.45	1.0000	0.104
298.65	1.0000	0.119
302.45	1.0000	0.138
306.75	1.0000	0.163
310.25	1.0000	0.189
317.05	1.0000	0.243
319.25	1.0000	0.277
319.65	1.0000	0.276
324.15	1.0000	0.340
325.75	1.0000	0.368

[a] $x_2^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

COMPONENTS:

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

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

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Domańska, U.

Polish J. Chem. 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature and Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_2^{(s)}$	x_1	T/K	$x_2^{(s)}$	x_1
284.05	0.0000	0.038	300.15	0.1956	0.0876
289.05	0.0000	0.045	303.75	0.1956	0.101
291.95	0.0000	0.050	308.45	0.1956	0.121
295.35	0.0000	0.058	311.20	0.1956	0.137
298.25	0.0000	0.066	316.35	0.1956	0.172
303.25	0.0000	0.077	318.95	0.1956	0.194
307.95	0.0000	0.091	323.40	0.1956	0.243
313.45	0.0000	0.113	338.25	0.1956	0.546
317.35	0.0000	0.140			
319.75	0.0000	0.156	282.55	0.4933	0.0556
323.55	0.0000	0.176	286.35	0.4933	0.0643
330.45	0.0000	0.228	291.55	0.4933	0.0786
			296.05	0.4933	0.0950
285.75	0.1956	0.0505	299.80	0.4933	0.110
291.15	0.1956	0.0619	304.35	0.4933	0.132
295.95	0.1956	0.0745	304.25	0.4933	0.162

(Continued next page)

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Reachim, Poland, was dried over phosphorous pentoxide and fractionally distilled to a final purity of 99.9+ %.

(3) Initial purity not specified, P.O.Ch., was dried over sodium carbonate and fractionally distilled to a final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0002 (compiler).
x_1: to 3 significant figs. (compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexane; C_6H_{14}; [110-54-3] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	Domańska, U. *Polish J. Chem.* 1981, *55*, 1715-1720. (numerical values obtained through personal communication with author.)
VARIABLES:	**PREPARED BY:**
Temperature and Solvent Composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

T/K	$x_2^{(s)}$	x_1
312.95	0.4933	0.190
318.45	0.4933	0.243
320.55	0.4933	0.265
331.05	0.4933	0.428
282.35	0.7994	0.0625
284.05	0.7994	0.0683
288.45	0.7994	0.0802
291.85	0.7994	0.0924
295.65	0.7994	0.107
300.25	0.7994	0.128
304.55	0.7994	0.154
309.75	0.7994	0.190
312.95	0.7994	0.221
315.25	0.7994	0.245
318.55	0.7994	0.284
327.75	0.7994	0.430
282.05	1.0000	0.063
286.35	1.0000	0.072
289.55	1.0000	0.084
289.85	1.0000	0.082
292.45	1.0000	0.094
295.45	1.0000	0.104
298.65	1.0000	0.119
302.45	1.0000	0.138
306.75	1.0000	0.163
310.25	1.0000	0.189
317.05	1.0000	0.243
319.25	1.0000	0.277
319.65	1.0000	0.276
324.15	1.0000	0.340
325.75	1.0000	0.368

[a] $x_2^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

COMPONENTS:

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

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

(3) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

ORIGINAL MEASUREMENTS:

Domańska, U.

Polish J. Chem. 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature and Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_2^{(s)}$	x_1	T/K	$x_2^{(s)}$	x_1
282.30	0.0000	0.054	296.75	0.1000	0.0947
286.35	0.0000	0.062	299.55	0.1000	0.108
290.35	0.0000	0.073	304.55	0.1000	0.122
296.05	0.0000	0.086	307.25	0.1000	0.137
299.95	0.0000	0.101	310.55	0.1000	0.154
305.75	0.0000	0.120	314.45	0.1000	0.180
310.85	0.0000	0.147	320.05	0.1000	0.230
314.95	0.0000	0.175	321.75	0.1000	0.253
318.95	0.0000	0.201	327.85	0.1000	0.319
321.45	0.0000	0.224	335.55	0.1000	0.487
331.55	0.0000	0.368			
			282.75	0.4979	0.0677
281.55	0.1000	0.0528	287.90	0.4979	0.0820
284.65	0.1000	0.0597	293.85	0.4979	0.103
288.25	0.1000	0.0681	299.15	0.4979	0.125
292.85	0.1000	0.0789	306.80	0.4979	0.169
			312.55	0.4979	0.218

(Continued next page)

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Reachim, Poland, was dried over phosphorous pentoxide and fractionally distilled to a final purity of 99.9+ %.

(3) Initial purity not specified, Reachim, was dried over sodium carbonate and distilled to final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0002 (compiler).
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexane; C_6H_{14}; [110-54-3] (3) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	Domańska, U. *Polish J. Chem.* 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)
VARIABLES:	**PREPARED BY:**
Temperature and Solvent Composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

T/K	$x_2^{(s)}$	x_1	*T*/K	$x_2^{(s)}$	x_1
318.55	0.4979	0.271	279.85	0.8998	0.0601
321.95	0.4979	0.313	283.75	0.8998	0.0706
325.75	0.4979	0.363	289.95	0.8998	0.0887
334.35	0.4979	0.539	295.75	0.8998	0.115
			301.05	0.8998	0.139
283.95	0.6994	0.0722	308.05	0.8998	0.184
290.00	0.6994	0.0900	313.05	0.8998	0.228
294.35	0.6994	0.106	316.85	0.8998	0.271
298.55	0.6994	0.125	321.45	0.8998	0.333
303.85	0.6994	0.153	324.65	0.8998	0.383
309.25	0.6994	0.194	327.55	0.8998	0.433
315.65	0.6994	0.253			
319.95	0.6994	0.309	282.05	1.0000	0.063
323.95	0.6994	0.368	286.35	1.0000	0.072
330.45	0.6994	0.482	289.55	1.0000	0.084
334.95	0.6994	0.581	289.85	1.0000	0.082
281.45	0.7999	0.0631	292.45	1.0000	0.092
285.50	0.7999	0.0755	295.45	1.0000	0.104
291.05	0.7999	0.0939	298.65	1.0000	0.119
293.55	0.7999	0.104	302.45	1.0000	0.138
300.05	0.7999	0.133	306.75	1.0000	0.163
305.00	0.7999	0.162	310.25	1.0000	0.189
308.95	0.7999	0.191	317.05	1.0000	0.243
311.35	0.7999	0.213	319.25	1.0000	0.277
315.25	0.7999	0.249	319.65	1.0000	0.276
318.60	0.7999	0.294	324.15	1.0000	0.340
321.45	0.7999	0.343	325.75	1.0000	0.368
325.25	0.7999	0.394			
332.95	0.7999	0.543			

[a] $x_2^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

COMPONENTS:

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

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

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Domańska, U.

Polish J. Chem. 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature and Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_2^{(s)}$	x_1	T/K	$x_2^{(s)}$	x_1
280.95	0.0000	0.069	284.25	0.2515	0.0787
284.35	0.0000	0.077	288.55	0.2515	0.0907
286.75	0.0000	0.084	292.05	0.2515	0.103
289.95	0.0000	0.092	296.25	0.2515	0.119
291.95	0.0000	0.099	299.35	0.2515	0.136
294.15	0.0000	0.108	305.30	0.2515	0.161
295.55	0.0000	0.116	309.85	0.2515	0.193
298.55	0.0000	0.124	314.55	0.2515	0.226
302.35	0.0000	0.139	320.15	0.2515	0.286
305.15	0.0000	0.153	325.25	0.2515	0.349
308.25	0.0000	0.169	335.05	0.2515	0.528
311.95	0.0000	0.194			
315.45	0.0000	0.221	280.05	0.5000	0.0668
317.45	0.0000	0.240	284.40	0.5000	0.0785
320.65	0.0000	0.267	287.85	0.5000	0.0890
323.35	0.0000	0.299	290.75	0.5000	0.100
325.95	0.0000	0.328	294.25	0.5000	0.114
331.55	0.0000	0.422	296.80	0.5000	0.125

(Continued next page)

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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 $^{\circ}$C.

(2) Initial purity not specified, Reachim, Poland, was dried over phosphorous pentoxide and fractionally distilled to a final purity of 99.9+ %.

(3) Initial purity not specified, Koch-Light, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0002 (compiler).
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexane; C_6H_{14}; [110-54-3] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	Domańska, U. *Polish J. Chem.* 1981, *55*, 1715-1720. (numerical values obtained through personal communication with author.)
VARIABLES:	**PREPARED BY:**
Temperature and Solvent Composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

T/K	$x_2^{(s)}$	x_1	T/K	$x_2^{(s)}$	x_1
298.75	0.5000	0.134	306.75	1.0000	0.163
302.65	0.5000	0.153	310.25	1.0000	0.189
306.20	0.5000	0.175	317.05	1.0000	0.243
309.05	0.5000	0.195	319.25	1.0000	0.277
312.95	0.5000	0.226	319.65	1.0000	0.276
316.30	0.5000	0.258	324.15	1.0000	0.340
320.80	0.5000	0.308	325.75	1.0000	0.368
327.95	0.5000	0.417			
283.35	0.8000	0.0724			
286.95	0.8000	0.0841			
290.35	0.8000	0.0963			
295.35	0.8000	0.116			
299.45	0.8000	0.135			
303.30	0.8000	0.158			
306.05	0.8000	0.177			
309.45	0.8000	0.199			
312.25	0.8000	0.224			
315.45	0.8000	0.257			
317.55	0.8000	0.283			
320.05	0.8000	0.317			
323.35	0.8000	0.359			
332.75	0.8000	0.543			
282.05	1.0000	0.063			
286.35	1.0000	0.072			
289.55	1.0000	0.084			
289.85	1.0000	0.082			
292.45	1.0000	0.094			
295.45	1.0000	0.104			
298.65	1.0000	0.119			
302.45	1.0000	0.138			

[a] $x_2^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
310.35	0.0000	0.3964	335.4	0.3000	0.7054
315.55	0.0000	0.4494	344.0	0.3000	0.8382
323.45	0.0000	0.5391			
334.35	0.0000	0.6885	297.6	1.0000	0.3032
344.15	0.0000	0.8422	325.3	1.0000	0.5748
			333.2	1.0000	0.6808
303.7	0.3000	0.3421	337.2	1.0000	0.7422
315.0	0.3000	0.4525	344.4	1.0000	0.8570
324.7	0.3000	0.5619			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLauglin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
300.15	0.0000	0.1597	341.3	0.3000	0.7832
308.25	0.0000	0.2254	347.2	0.3000	0.8984
315.15	0.0000	0.3025			
325.45	0.0000	0.4612	297.6	1.0000	0.3032
333.15	0.0000	0.6073	325.3	1.0000	0.5748
343.05	0.0000	0.8082	333.2	1.0000	0.6808
			337.2	1.0000	0.7422
301.1	0.3000	0.2763	344.4	1.0000	0.8570
314.8	0.3000	0.4083			
322.2	0.3000	0.5047			
330.8	0.3000	0.6189			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
310.35	0.0000	0.3964	336.2	0.3000	0.7142
315.55	0.0000	0.4494	344.4	0.3000	0.8424
323.45	0.0000	0.5391			
334.35	0.0000	0.6885	303.2	1.0000	0.3588
344.15	0.0000	0.8422	318.2	1.0000	0.5011
			322.7	1.0000	0.5510
303.9	0.3000	0.3433	336.8	1.0000	0.7372
314.8	0.3000	0.4476	341.1	1.0000	0.8053
324.6	0.3000	0.5520	348.1	1.0000	0.9167

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data, 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data, 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Eng. Chem. Fundam., 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	*T*/K	$x_3^{(s)}$	x_1
300.15	0.0000	0.1597	337.9	0.3000	0.7202
308.25	0.0000	0.2254	347.8	0.3000	0.8998
315.15	0.0000	0.3025			
325.45	0.0000	0.4612	303.2	1.0000	0.3588
333.15	0.0000	0.6073	318.2	1.0000	0.5011
343.05	0.0000	0.8082	322.7	1.0000	0.5510
			336.8	1.0000	0.7372
308.2	0.3000	0.2880	341.1	1.0000	0.8053
312.9	0.3000	0.3593	348.1	1.0000	0.9167
319.7	0.3000	0.4430			
327.1	0.3000	0.5486			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
303.2	0.0000	0.3588	323.0	0.3000	0.6737
318.2	0.0000	0.5011	346.0	0.3000	0.8696
322.7	0.0000	0.5510			
336.8	0.0000	0.7372	297.6	1.0000	0.3032
341.1	0.0000	0.8053	325.3	1.0000	0.5748
348.1	0.0000	0.9167	333.2	1.0000	0.6808
			337.2	1.0000	0.7422
303.8	0.3000	0.3561	344.4	1.0000	0.8570
306.7	0.3000	0.3822			
317.8	0.3000	0.4911			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$x_3^{(s)}$	x_3[b]	x_1
0.0000	0.0000	0.2926
0.1505	0.1064	0.2930
0.4089	0.2892	0.2928
0.5872	0.4151	0.2931
0.8400	0.5930	0.2940
1.0000	0.7054	0.2946

[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.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained by extrapolation of a calibration plot of refractive index vs. solute concentration to the refractive index of the saturated solution. Attainment of equilibrium was verified by repetitive measurements several days later.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over calcium hydride and distilled to a final purity of 99.9 %.

(3) Spectroquality, Matheson, Coleman and Bell dried over sodium and distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_3^{(s)}$: ± 0.0001.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
306.6	0.0000	0.3635	339.6	0.5000	0.7580
311.7	0.0000	0.4141	345.1	0.5000	0.8555
318.4	0.0000	0.4820			
323.7	0.0000	0.5506	302.9	1.0000	0.2262
330.1	0.0000	0.6272	307.7	1.0000	0.2705
			311.7	1.0000	0.3181
308.8	0.5000	0.3506	319.0	1.0000	0.3960
318.5	0.5000	0.4529	324.3	1.0000	0.4703
324.9	0.5000	0.5336	329.7	1.0000	0.5623
335.0	0.5000	0.6801	335.6	1.0000	0.6725

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

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.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

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

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

(3) Diiodomethane; CH_2I_2; [75-11-6]

ORIGINAL MEASUREMENTS:

Domańska, U.

Polish J. Chem. 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature and Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_2^{(s)}$	x_1	T/K	$x_2^{(s)}$	x_1
321.85	0.0000	0.4381	312.95	0.4920	0.4091
319.10	0.0000	0.3967	302.75	0.4920	0.3056
313.00	0.0000	0.3142	297.75	0.4920	0.2695
307.00	0.0000	0.2485	294.95	0.4920	0.2482
301.85	0.0000	0.2017	289.60	0.4920	0.2127
295.85	0.0000	0.1593	284.80	0.4920	0.1846
291.00	0.0000	0.1310	281.75	0.4920	0.1662
286.55	0.0000	0.1094			
281.75	0.0000	0.0904	315.25	0.7000	0.4134
			303.15	0.7000	0.2962
315.15	0.3069	0.4132	299.15	0.7000	0.2680
302.60	0.3069	0.2960	296.95	0.7000	0.2515
299.20	0.3069	0.2688	295.05	0.7000	0.2411
296.95	0.3069	0.2517	290.95	0.7000	0.2090
295.15	0.3069	0.2398	287.35	0.7000	0.1853
291.00	0.3069	0.2092	280.65	0.7000	0.1530
287.45	0.3069	0.1859			
280.85	0.3069	0.1533			

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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 ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, P.O.Ch., Gliwice, was dried over sodium metal and fractionally distilled to a final purity of 99.9+ %.

(3) Initial purity not specified, Chemapol, Czechoslovakia, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0002 (compiler).
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Diiodomethane; CH_2I_2; [75-11-6]	Domańska, U. *Polish J. Chem.* <u>1981</u>, *55*, 1715-1720. (numerical values obtained through personal communication with author.)
VARIABLES:	**PREPARED BY:**
Temperature and Solvent Composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

T/K	$x_2^{(s)}$	x_1
326.75	1.0000	0.485
319.40	1.0000	0.358
318.25	1.0000	0.346
306.75	1.0000	0.212
306.35	1.0000	0.208
301.85	1.0000	0.172
301.55	1.0000	0.170
295.95	1.0000	0.134
295.50	1.0000	0.131

[a] $x_2^{(s)}$: initial mole fraction of the binary solvent mixture; x_1: mole fraction solubility of the solute.

COMPONENTS:

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

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

(3) Diethyl ether; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.247
0.161	0.121	0.247
0.386	0.297	0.231
0.656	0.483	0.264
1.000	0.660	0.340

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

(2) Carbon disulfide; CS_2; [75-15-0]

(3) Diethyl ether; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$x_2^{(s),b}$	x_2^{b}	x_1^{b}
0.000	0.000	0.247
0.231	0.162	0.298
0.455	0.311	0.317
0.728	0.499	0.314
1.000	0.714	0.286

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] 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.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

(3) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$x_2^{(s)}$: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

J. Chem. Eng. Data 1990, *35*, 244-246.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C		t = 15.0 °C	
$m_2^{(s)}$	c_1	$m_2^{(s)}$	c_1
0.0000	0.000135	0.0000	0.000190
1.3193	0.000162	1.3193	0.000236
2.5165	0.000185	2.5165	0.000282
3.8190	0.000212	3.8190	0.000328
4.9828	0.000263	4.9828	0.000426
6.2146	0.000324	6.2146	0.000546
t = 10.0 °C		t = 20.0 °C	
0.0000	0.000158	0.0000	0.000224
1.3193	0.000193	1.3193	0.000296
2.5165	0.000220	2.5165	0.000336
3.8190	0.000268	3.8190	0.000392
4.9828	0.000323	4.9828	0.000525
6.2146	0.000417	6.2146	0.000668

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) Analysis grade, 99.7 %, E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

J. Chem. Eng. Data 1990, *35*, 244-246.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303
and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C		t = 35.0 °C	
$m_2^{(s)}$	c_1	$m_2^{(s)}$	c_1
0.0000	0.000263	0.0000	0.000371
1.3193	0.000344	1.3193	0.000462
2.5165	0.000398	2.5165	0.000547
3.8190	0.000495	3.8190	0.000697
4.9828	0.000631	4.9828	0.000871
6.2146	0.000841	6.2146	0.001306

t = 30.0 °C	
0.0000	0.000324
1.3193	0.000407
2.5165	0.000492
3.8190	0.000588
4.9828	0.000785
6.2146	0.001085

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methanol; CH_4O; [67-56-1] (3) Water; H_2O; [7732-18-5]	Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. *J. Chem. Eng. Data* 1989, *34*, 438-443.
VARIABLES:	**PREPARED BY:**
$T/K = 298$, Solvent Composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25\ °C$

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.01	4.28×10^{-6}
0.03	4.94×10^{-6}
0.05	5.29×10^{-6}
0.10	6.96×10^{-6}
1.00	2.35×10^{-2}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.9 %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.01	4.53×10^{-6}
0.03	4.80×10^{-6}
0.05	5.80×10^{-6}
0.10	8.00×10^{-6}
0.25	3.02×10^{-5}
0.50	7.38×10^{-4}
0.75	5.56×10^{-3}
1.00	3.98×10^{-2}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.9+ %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

J. Chem. Eng. Data 1990, *35*, 244-246.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000135
0.9216	0.000165
1.3455	0.000199
1.8501	0.000237
2.3816	0.000305
2.9590	0.000457

t = 15.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000190
0.9216	0.000263
1.3455	0.000322
1.8501	0.000370
2.3816	0.000531
2.9590	0.000741

t = 10.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000158
0.9216	0.000204
1.3455	0.000243
1.8501	0.000313
2.3816	0.000421
2.9590	0.000603

t = 20.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000224
0.9216	0.000316
1.3455	0.000389
1.8501	0.000484
2.3816	0.000662
2.9590	0.000832

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) Analysis grade, 99.7 %, E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Water; H_2O; [7732-18-5]	Perez-Tejeda, P.; Yanes, C.; Maestre, A. *J. Chem. Eng. Data* <u>1990</u>, *35*, 244-246.
VARIABLES:	**PREPARED BY:**
T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000263
0.9216	0.000398
1.3455	0.000477
1.8501	0.000616
2.3816	0.000828
2.9590	0.001202

t = 35.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000371
0.9216	0.000582
1.3455	0.000702
1.8501	0.000916
2.3816	0.001265
2.9590	0.001862

t = 30.0 °C

0.0000	0.000324
0.9216	0.000497
1.3455	0.000596
1.8501	0.000749
2.3816	0.001036
2.9590	0.001480

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25\ ^{\circ}C$

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.01	4.57×10^{-6}
0.03	5.44×10^{-6}
0.05	6.76×10^{-6}
0.10	1.08×10^{-5}
1.00	5.05×10^{-2}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.5 %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

J. Chem. Eng. Data 1990, *35*, 244-246.

VARIABLES:

T/K = 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 10.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000158
0.1631	0.000164
0.3478	0.000174
0.5507	0.000219
0.7166	0.000245

t = 15.0 °C

0.0000	0.000190
0.1631	0.000206
0.3478	0.000224
0.5507	0.000285
0.7166	0.000301

t = 20.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000224
0.1631	0.000244
0.3478	0.000279
0.5507	0.000345
0.7166	0.000353

t = 25.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000263
0.1631	0.000295
0.3478	0.000345
0.5507	0.000403
0.7166	0.000447

t = 30.0 °C

0.0000	0.000324
0.1631	0.000365
0.3478	0.000415
0.5507	0.000472
0.7166	0.000532

t = 35.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000371
0.1631	0.000426
0.3478	0.000503
0.5507	0.000571
0.7166	0.000612

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) Analysis grade, 99.7 %, E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:

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

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25\ ^\circ C$

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.01	4.55×10^{-6}
0.03	6.13×10^{-6}
0.05	6.37×10^{-6}
0.07	9.56×10^{-6}
1.00	6.66×10^{-2}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.9 %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

$T/K = 298$, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25\ ^\circ C$

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.005	4.16×10^{-6}
0.01	4.52×10^{-6}
0.02	5.60×10^{-6}
1.00	8.11×10^{-2}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99 %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

J. Chem. Eng. Data 1990, *35*, 244-246.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES^a

t = 5.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000135
0.3109	0.000151
0.7036	0.000180
1.0122	0.000193
1.3549	0.000224
1.6883	0.000250

t = 10.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000158
0.3109	0.000182
0.7036	0.000215
1.0122	0.000233
1.3549	0.000269
1.6883	0.000302

t = 15.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000190
0.3109	0.000224
0.7036	0.000262
1.0122	0.000295
1.3549	0.000331
1.6883	0.000380

t = 20.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000224
0.3109	0.000263
0.7036	0.000297
1.0122	0.000338
1.3549	0.000379
1.6883	0.000447

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) Analysis grade, 99.5 %, E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:

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

(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

J. Chem. Eng. Data 1990, *35*, 244-246.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000263
0.3109	0.000316
0.7036	0.000349
1.0122	0.000407
1.3549	0.000467
1.6883	0.000524

t = 35.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000371
0.3109	0.000437
0.7036	0.000498
1.0122	0.000563
1.3549	0.000667
1.6883	0.000763

t = 30.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000324
0.3109	0.000372
0.7036	0.000438
1.0122	0.000495
1.3549	0.000567
1.6883	0.000663

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:

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

(2) 2-Propanone; C_3H_6O; [67-64-1]

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.01	4.56×10^{-6}
0.03	6.64×10^{-6}
0.05	8.14×10^{-6}
0.10	1.53×10^{-5}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and liquid chromatograph with uv detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and the absorbances of a constant μl volume was measured at 254 nm by use of Waters HPLC, with spherisorb S-5-O-DS and 50/50 acetonitrile-water mixture (by volume) serving as the stationary and mobile phases, respectively.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.5 %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) 2-Butanone; C_4H_8O; [78-93-3]

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

T/K = 298, Solvent Composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25 °C

$\phi_2^{(s)}$	x_1
0.00	4.11×10^{-6}
0.01	4.65×10^{-6}
0.03	6.78×10^{-6}
0.05	1.09×10^{-5}
0.10	2.15×10^{-5}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and liquid chromatograph with uv detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solutions were removed and the absorbances of a constant μl volume was measured at 254 nm by use of Waters HPLC, with spherisorb S-5-O-DS and 50/50 acetonitrile-water mixture (by volume) serving as the stationary and mobile phases, respectively.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.7 %, source not given.

(3) Purity and source not given, was pretreated by distillation and passage through a Milli-Q water purification system affixed with a 0.22 μm Organex-Q filter.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
$\phi_2^{(s)}$: ± 0.005 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) Dimethyl sulfoxide; C_2H_6OS; [67-88-5]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

Thermochim. Acta 1990, *157*, 105-112.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C		t = 15.0 °C	
$m_2^{(s)}$	c_1	$m_2^{(s)}$	c_1
0.0000	0.000135	0.0000	0.000191
0.6556	0.000162	0.6556	0.000263
1.3600	0.000224	1.3600	0.000347
2.2120	0.000302	2.2120	0.000490
2.9450	0.000398	2.9450	0.000589
4.0890	0.000525	4.0890	0.000832

t = 10.0 °C		t = 20.0 °C	
0.0000	0.000158	0.0000	0.000224
0.6556	0.000214	0.6556	0.000324
1.3600	0.000282	1.3600	0.000417
2.2120	0.000380	2.2120	0.000575
2.9450	0.000479	2.9450	0.000741
4.0890	0.000661	4.0890	0.00100

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) p.a., E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:

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

(2) Dimethyl sulfoxide; C_2H_6OS; [67-88-5]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

Thermochim. Acta <u>1990</u>, *157*, 105-112.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000263
0.6556	0.000355
1.3600	0.000479
2.2120	0.000676
2.9450	0.000891
4.0890	0.00123

t = 35.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000371
0.6556	0.000562
1.3600	0.000661
2.2120	0.00105
2.9450	0.00132
4.0890	0.00178

t = 30.0 °C

0.0000	0.000324
0.6556	0.000468
1.3600	0.000603
2.2120	0.000851
2.9450	0.00112
4.0890	0.00148

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:

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

(2) N,N-Dimethylformamide; C_3H_7NO; [68-12-2]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

Thermochim. Acta 1990, *157*, 105-112.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000135
0.8371	0.000309
1.5621	0.000501
2.4262	0.000813
3.3996	0.00138
4.5362	0.00199

t = 10.0 °C

0.0000	0.000158
0.8371	0.000355
1.5621	0.000603
2.4262	0.00100
3.3996	0.00162
4.5362	0.00245

t = 15.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000191
0.8371	0.000398
1.5621	0.000724
2.4262	0.00117
3.3996	0.00195
4.5362	0.00309

t = 20.0 °C

0.0000	0.000224
0.8371	0.000513
1.5621	0.000891
2.4262	0.00148
3.3996	0.00240
4.5362	0.00380

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) p.a., E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) N,N-Dimethylformamide; C_2H_7NO; [68-12-2] (3) Water; H_2O; [7732-18-5]	Perez-Tejeda, P.; Yanes, C.; Maestre, A. *Thermochim. Acta* 1990, *157*, 105-112.
VARIABLES:	**PREPARED BY:**
T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t =25.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000263
0.8371	0.000589
1.5621	0.00105
2.4262	0.00178
3.3996	0.00288
4.5362	0.00457

t = 35.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000371
0.8371	0.000871
1.5621	0.00158
2.4262	0.00263
3.3996	0.00427
4.5362	0.00692

t = 30.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000324
0.8371	0.000708
1.5621	0.00129
2.4262	0.00214
3.3996	0.00347
4.5362	0.00562

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:

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

(2) Acetonitrile; C_2H_3N; [75-05-8]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

Thermochim. Acta 1990, *157*, 105-112.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000135
0.6465	0.000126
1.4049	0.000191
2.7077	0.000282
4.3037	0.000562
6.1142	0.00129

t = 10.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000158
0.6465	0.000162
1.4049	0.000229
2.7077	0.000380
4.3037	0.000708
6.1142	0.00151

t = 15.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000191
0.6465	0.000219
1.4049	0.000275
2.7077	0.000512
4.3037	0.000871
6.1142	0.00166

t = 20.0 °C

$m_2^{(s)}$	c_1
0.0000	0.000224
0.6465	0.000282
1.4049	0.000347
2.7077	0.000562
4.3037	0.00107
6.1142	0.00224

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) p.a., E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:

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

(2) Acetonitrile; C_2H_3N; [75-05-8]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

Thermochim. Acta 1990, *157*, 105-112.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C		t = 35.0 °C	
$m_2^{(s)}$	c_1	$m_2^{(s)}$	c_1
0.0000	0.000263	0.0000	0.000371
0.6465	0.000295	0.6465	0.000512
1.4049	0.000398	1.4049	0.000617
2.7077	0.000692	2.7077	0.000933
4.3037	0.00142	4.3037	0.00182
6.1142	0.00309	6.1142	0.00363

t = 30.0 °C

0.0000	0.000324
0.6465	0.000398
1.4049	0.000501
2.7077	0.000832
4.3037	0.00158
6.1142	0.00324

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:

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

(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

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

ORIGINAL MEASUREMENTS:

Huot, J.-Y.; Page, M.; Jolicoeur, C.

J. Solution Chem. 1991, *20*, 1093-1112.

VARIABLES:

T/K = 278, 288, 298, 308 and 318
Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C		*t* = 15.0 °C	
$x_2^{(s)}$	c_1	$x_2^{(s)}$	c_1
0.00	0.0000119	0.00	0.000158
0.02	0.000137	0.02	0.000184
0.05	0.000167	0.05	0.000237
0.08	0.000207	0.08	0.000311
0.10	0.000244	0.10	0.000372
0.15	0.000412	0.15	0.000614
0.20	0.000651	0.20	0.001004
0.25	0.00106	0.25	0.00156
0.30	0.00152	0.30	0.00233
0.35	0.00235	0.35	0.00354
0.40	0.00346	0.40	0.00505
0.50	0.00705	0.50	0.00965
0.60	0.0118	0.60	0.0171
0.80	0.0270	0.80	0.0396
0.997	0.0510	0.997	0.0696

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, precision thermometer, ultraviolet/visible spectrophotometer, and a peristaltic pump.

Binary solvent mixtures were prepared by weight. Relative solubilities were determined with a packed-column method. Peristaltic pump continuously circulated liquid solution through temperature controlled naphthalene-packed column until equilibrium was obtained. Aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 278 nm. Cell pathlengths and dilution ratios were varied in order to keep measured absorbances below unity.

Solubilities computed by compiler from published absorbance data using an extinction coefficient of ϵ = 57000 dm^2 mol^{-1}, given in the original paper.

SOURCE AND PURITY OF MATERIALS:

(1) AR Grade, J.T. Baker, Inc. Phillipsburg, New Jersey, USA, was used as received.

(2) Fisher Certified, Fisher Scientific Company, Pittsburgh, Pennsylvania, USA, was used as received.

(3) Purity and source not given, was distilled and deionized on a Millipore ion exchanger Milli-Q system.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
$x_2^{(s)}$: ± 0.005 (compiler).
c_1: ± 2 - 5 % (relative error), depending upon dilutions used.

COMPONENTS:

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

(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

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

ORIGINAL MEASUREMENTS:

Huot, J.-Y.; Page, M.; Jolicoeur, C.

J. Solution Chem. 1991, *20*, 1093-1112.

VARIABLES:

T/K = 278, 288, 298, 308 and 318
Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C

$x_2^{(s)}$	c_1
0.00	0.000204
0.02	0.000249
0.05	0.000333
0.08	0.000454
0.10	0.000567
0.15	0.000907
0.20	0.00151
0.25	0.00232
0.30	0.00356
0.35	0.00525
0.40	0.00758
0.50	0.0135
0.60	0.0237
0.80	0.0500
0.997	0.0905

t = 45.0 °C

$x_2^{(s)}$	c_1
0.00	0.000391
0.02	0.000495
0.05	0.000698
0.08	0.000961
0.10	0.00120
0.15	0.00202
0.20	0.00330
0.25	0.00542
0.30	0.00796
0.35	0.0118
0.40	0.0165
0.50	0.0296
0.60	0.0458
0.80	0.0996
0.997	0.168

t = 35.0 °C

0.00	0.000288
0.02	0.000358
0.05	0.000486
0.08	0.000653
0.10	0.000812
0.15	0.00136
0.20	0.00223
0.25	0.00356
0.30	0.00542
0.35	0.00786
0.40	0.0111
0.50	0.0196
0.60	0.0325
0.80	0.0705
0.997	0.125

[a] $x_2^{(s)}$: initial mole fraction composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

COMPONENTS:

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

(2) Urea; CH_4N_2O; [57-13-6]

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

ORIGINAL MEASUREMENTS:

Perez-Tejeda, P.; Yanes, C.; Maestre, A.

Thermochim. Acta 1990, *157*, 105-112.

VARIABLES:

T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 5.0 °C		t = 15.0 °C	
$m_2^{(s)}$	c_1	$m_2^{(s)}$	c_1
0.0000	0.000135	0.0000	0.000191
0.8767	0.000155	0.8767	0.000213
1.6257	0.000179	1.6257	0.000257
3.0076	0.000218	3.0076	0.000309
4.1028	0.000263	4.1028	0.000363
5.3722	0.000288	5.3722	0.000426
t = 10.0 °C		t = 20.0 °C	
0.0000	0.000158	0.0000	0.000224
0.8767	0.000191	0.8767	0.000263
1.6257	0.000209	1.6257	0.000302
3.0076	0.000257	3.0076	0.000372
4.1028	0.000309	4.1028	0.000447
5.3722	0.000347	5.3722	0.000525

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Binary solvent mixtures were prepared by weight. Solid naphthalene and solvent were placed in stoppered pyrex flasks and allowed to equilibrate at a constant temperature for 50 minutes. Solutions were stirred at 25,000 rpm for 8 minutes. After equilibrium was obtained aliquots of saturated solutions were removed and quantitatively diluted for spectrophotometric analysis at 275 nm.

SOURCE AND PURITY OF MATERIALS:

(1) puriss, 99 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, recrystallized from ethanol.

(2) p.a., E. Merck, Darmstadt, Germany, was used as received.

(3) Purity and source not given, was distilled twice using an all-glass apparatus.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
$m_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 2 % (relative error, compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Urea; CH_4N_2O; [57-13-6] (3) Water; H_2O; [7732-18-5]	Perez-Tejeda, P.; Yanes, C.; Maestre, A. *Thermochim. Acta* 1990, *157*, 105-112.
VARIABLES:	**PREPARED BY:**
T/K = 278, 283, 288, 293, 298, 303 and 308, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a] (Continued)

t = 25.0 °C		t = 35.0 °C	
$m_2^{(s)}$	c_1	$m_2^{(s)}$	c_1
0.0000	0.000263	0.0000	0.000371
0.8767	0.000302	0.8767	0.000417
1.6257	0.000339	1.6257	0.000513
3.0076	0.000427	3.0076	0.000589
4.1028	0.000490	4.1028	0.000741
5.3722	0.000589	5.3722	0.000933

t = 30.0 °C

0.0000	0.000324
0.8767	0.000372
1.6257	0.000427
3.0076	0.000501
4.1028	0.000617
5.3722	0.000692

[a] $m_2^{(s)}$: initial molal (mol kg^{-1}) composition of the binary solvent mixture; c_1 is the molar solubility (mol dm^{-3}) of the solute.

PHENANTHRENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

None

II. Alkane + Aromatic Hydrocarbon

cyclohexane + benzene

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

benzene + pyridine
cyclohexane + pyridine
benzene + thiophene
cyclohexane + thiophene
thiophene + pyridine
1,2,3,4-tetrahydronaphthalene + decahydronaphthalene

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.65	0.0000	0.0606	343.55	0.5000	0.5629
313.85	0.0000	0.0819	360.85	0.5000	0.8177
319.65	0.0000	0.1093			
321.85	0.0000	0.1228	307.95	0.7000	0.2041
325.85	0.0000	0.1530	314.65	0.7000	0.2567
333.25	0.0000	0.2430	324.55	0.7000	0.3521
339.55	0.0000	0.3568	351.55	0.7000	0.6910
			362.65	0.7000	0.8556
312.25	0.3000	0.1469			
320.25	0.3000	0.2123	312.75	1.0000	0.2815
326.85	0.3000	0.2800	316.75	1.0000	0.3128
353.75	0.3000	0.7018	325.25	1.0000	0.3958
360.65	0.3000	0.8147	334.75	1.0000	0.4949
			341.85	1.0000	0.5771
305.35	0.5000	0.1503	342.15	1.0000	0.5792
318.65	0.5000	0.2503			
327.25	0.5000	0.3415			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
312.75	0.0000	0.2815	299.8	1.0000	0.2459
316.75	0.0000	0.3128	307.7	1.0000	0.3011
325.25	0.0000	0.3958	314.4	1.0000	0.3513
334.75	0.0000	0.4949	316.6	1.0000	0.3690
341.85	0.0000	0.5771	323.4	1.0000	0.4283
342.15	0.0000	0.5792	342.8	1.0000	0.6170
			349.6	1.0000	0.6961
313.4	0.3000	0.2983	355.6	1.0000	0.7651
325.2	0.3000	0.3993	361.0	1.0000	0.8349
334.3	0.3000	0.5014	366.5	1.0000	0.9111
342.6	0.3000	0.5968			
351.8	0.3000	0.7033			
359.2	0.3000	0.8075			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.65	0.0000	0.0606	345.7	0.3000	0.6059
313.85	0.0000	0.0819	355.4	0.3000	0.7267
319.65	0.0000	0.1093			
321.85	0.0000	0.1228	299.8	1.0000	0.2459
325.85	0.0000	0.1530	307.7	1.0000	0.3011
333.25	0.0000	0.2430	314.3	1.0000	0.3513
339.55	0.0000	0.3568	316.6	1.0000	0.3690
			323.4	1.0000	0.4283
325.6	0.3000	0.3442	342.8	1.0000	0.6170
328.5	0.3000	0.3830	349.6	1.0000	0.6961
338.2	0.3000	0.5036	355.6	1.0000	0.7651
			361.0	1.0000	0.8349
			366.5	1.0000	0.9111

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
312.75	0.0000	0.2815	347.8	0.3000	0.6550
316.75	0.0000	0.3128	356.5	0.3000	0.7673
325.25	0.0000	0.3958			
334.75	0.0000	0.4949	299.4	1.0000	0.2379
341.85	0.0000	0.5771	304.9	1.0000	0.2742
342.15	0.0000	0.5792	310.0	1.0000	0.3146
			321.2	1.0000	0.4016
306.5	0.3000	0.2479	340.9	1.0000	0.5907
311.6	0.3000	0.2888	348.3	1.0000	0.6757
316.1	0.3000	0.3223	355.0	1.0000	0.7541
324.8	0.3000	0.4024			
331.5	0.3000	0.4710			
338.7	0.3000	0.5455			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
307.65	0.0000	0.0606	340.3	0.3000	0.5165
313.85	0.0000	0.0819	351.6	0.3000	0.7007
319.65	0.0000	0.1093			
321.85	0.0000	0.1228	299.4	1.0000	0.2379
325.85	0.0000	0.1530	304.9	1.0000	0.2742
333.25	0.0000	0.2430	310.0	1.0000	0.3146
339.55	0.0000	0.3568	321.2	1.0000	0.4016
			340.9	1.0000	0.5907
301.9	0.3000	0.1168	348.3	1.0000	0.6757
309.2	0.3000	0.1558	355.0	1.0000	0.7541
316.5	0.3000	0.2096			
323.3	0.3000	0.2759			
330.7	0.3000	0.3731			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.
J. Chem. Eng. Data 1985, *30*, 403-409.

Coon, J.E.; Troth, M.; McLaughlin, E.
J. Chem. Eng. Data 1987, *32*, 233-240.

Choi, P.B.; McLaughlin, E.
Ind. Chem. Eng. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
299.4	0.0000	0.2379	299.8	1.0000	0.2459
304.9	0.0000	0.2742	307.7	1.0000	0.3011
310.0	0.0000	0.3146	314.3	1.0000	0.3513
321.2	0.0000	0.4016	316.6	1.0000	0.3690
340.9	0.0000	0.5907	323.4	1.0000	0.4283
348.3	0.0000	0.6757	342.8	1.0000	0.6170
355.0	0.0000	0.7541	349.6	1.0000	0.6961
			355.6	1.0000	0.7651
308.3	0.3000	0.3038	361.0	1.0000	0.8349
309.7	0.3000	0.3136	366.5	1.0000	0.9111
327.7	0.3000	0.4599			
344.4	0.3000	0.6296			
351.0	0.3000	0.7157			
351.1	0.3000	0.7157			

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

(3) 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, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T/K	$x_3^{(s)}$	x_1	T/K	$x_3^{(s)}$	x_1
309.7	0.0000	0.2843	348.6	0.5000	0.6540
316.2	0.0000	0.3343	352.2	0.5000	0.6973
325.8	0.0000	0.4175			
333.1	0.0000	0.4887	314.4	1.0000	0.1593
340.6	0.0000	0.5681	320.1	1.0000	0.2020
			326.2	1.0000	0.2554
312.7	0.5000	0.2522	331.9	1.0000	0.3283
324.4	0.5000	0.3530	337.4	1.0000	0.4030
333.0	0.5000	0.4583	341.2	1.0000	0.4751
341.6	0.5000	0.5542	345.6	1.0000	0.5612

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute.

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 ampoules and placed in a constant temperature to equilibrate. Samples were rotated at a speed of 0.25 rps while the bath temperature was slowly increased by 0.1 K every 1200 seconds. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared. At least two measurements were performed for each mixture composition.

SOURCE AND PURITY OF MATERIALS:

(1) 98.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over activated alumina and then recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company.

(3) 99+ %, Aldrich Chemical Company, having an isomer ratio of 60.6 % cis and 39.4 % trans.

Components 2 and 3 were stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 0.0003.

PYRENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes

n-hexane + cyclohexane
n-heptane + cyclohexane
n-octane + cyclohexane
2,2,4-trimethylpentane + cyclohexane
cyclohexane + cyclooctane

II. Alkane + Aromatic Hydrocarbon

n-hexane + benzene
n-heptane + benzene
n-octane + benzene
cyclohexane + benzene
2,2,4-trimethylpentane + benzene
cyclooctane + benzene

III. Alkane + Ester

None

IV. Alkane + Ether

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

V. Alkane + Chloroalkane

n-hexane + 1,4-dichlorobutane
n-heptane + 1,4-dichlorobutane
n-octane + 1,4-dichlorobutane
cyclohexane + 1,4-dichlorobutane
methylcyclohexane + 1,4-dichlorobutane
2,2,4-trimethylpentane + 1,4-dichlorobutane

VI. Ether + Chloroalkane

None

VII. Miscellaneous

methylbenzene + 2-propanone
methylbenzene + ethanol
methylbenzene + pyridine

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00852
0.2195	0.2174	0.00942
0.4365	0.4321	0.01016
0.5513	0.5455	0.01049
0.6018	0.5954	0.01057
0.6503	0.6434	0.01066
0.7687	0.7604	0.01077
0.8300	0.8209	0.01099
1.0000	0.9891	0.01089

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) 99 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^\circ C$

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01101
0.1506	0.1489	0.01121
0.2572	0.2543	0.01145
0.4685	0.4631	0.01152
0.5682	0.5616	0.01156
0.6592	0.6516	0.01151
0.8382	0.8287	0.01134
1.0000	0.9891	0.01089

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(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.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 26.0$ °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01379
0.1751	0.1727	0.01369
0.2840	0.2802	0.01350
0.5005	0.4939	0.01314
0.5532	0.5460	0.01299
0.6063	0.5985	0.01281
0.6938	0.6852	0.01246
0.8577	0.8477	0.01171
1.0000	0.9891	0.01089

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00721
0.2874	0.2851	0.00803
0.4993	0.4949	0.00887
0.5579	0.5528	0.00909
0.6003	0.5947	0.00926
0.7007	0.6940	0.00958
0.7022	0.6954	0.00962
0.8533	0.8445	0.01027
1.0000	0.9891	0.01089

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(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.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Cyclooctane; C_8H_{16}; [292-64-8]	**ORIGINAL MEASUREMENTS:** Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1987, *32*, 60-62.
VARIABLES: T/K = 299, Solvent composition	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.01956
0.2387	0.2344	0.01780
0.4680	0.4606	0.01572
0.5624	0.5540	0.01489
0.6638	0.6544	0.01409
0.6655	0.6562	0.01400
0.8363	0.8258	0.01250
1.0000	0.9891	0.01089

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. <u>1987</u>, *16*, 179-187.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00852
0.1993	0.1965	0.01386
0.2833	0.2786	0.01676
0.4016	0.3927	0.02225
0.4977	0.4840	0.02756
0.6008	0.5804	0.03389
0.6824	0.6554	0.03961
0.8451	0.9489	0.05107
1.0000	0.9368	0.06316

[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 372 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.

(3) HPLC Grade, 99.9+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *16*, 179-187.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01101
0.2111	0.2076	0.01640
0.3091	0.3028	0.02049
0.5277	0.5113	0.03102
0.6219	0.5989	0.03702
0.7213	0.6899	0.04352
0.8627	0.8171	0.05280
1.0000	0.9368	0.06316

[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 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99.7+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *16*, 179-187.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01379
0.2031	0.1990	0.02028
0.3288	0.3207	0.02455
0.5434	0.5249	0.03398
0.6549	0.6287	0.04006
0.7355	0.7029	0.04428
0.8729	0.8255	0.05432
1.0000	0.9368	0.06316

[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 372 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.

(3) HPLC Grade, 99.9+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *16*, 179-187.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 26.0$ °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01089
0.2504	0.2452	0.02058
0.3502	0.3413	0.02541
0.4420	0.4282	0.03118
0.5524	0.5321	0.03680
0.6525	0.6245	0.04289
0.8196	0.7766	0.05243
1.0000	0.9368	0.06316

[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 372 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.

(3) HPLC Grade, 99.9+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2,2,4-Trimethylpentane; C_6H_{12}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *16*, 179-187.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00721
0.2301	0.2274	0.01177
0.3021	0.2980	0.01373
0.5482	0.5348	0.02446
0.6520	0.6314	0.03165
0.7444	0.7157	0.03854
0.8799	0.8345	0.05160
1.0000	0.9368	0.06316

[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 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Fisher Scientific, Pittsburgh, Pennsylvania, USA.

(3) HPLC Grade, 99.9+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *16*, 179-187.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01956
0.2007	0.1952	0.02763
0.2969	0.2873	0.03236
0.5031	0.4868	0.04327
0.6026	0.5731	0.04898
0.6982	0.6607	0.05371
0.8517	0.8007	0.05993
1.0000	0.9368	0.06316

[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 372 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.

(3) HPLC Grade, 99.9+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.0298
0.1879	0.1831	0.0255
0.2536	0.2475	0.0242
0.4650	0.4561	0.0190
0.5694	0.5598	0.0168
0.6635	0.6537	0.0148
0.8350	0.8256	0.0113
1.0000	0.9914	0.0086

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0112
0.1915	0.1888	0.0143
0.3678	0.3615	0.0170
0.4995	0.4896	0.0198
0.5744	0.5622	0.0213
0.7708	0.7512	0.0254
0.8733	0.8495	0.0273
1.0000	0.9702	0.0298

[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 372 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.

(3) Gold Label, 99+ %, 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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.0298
0.2133	0.2078	0.0259
0.3501	0.3419	0.0233
0.5155	0.5049	0.0205
0.6123	0.6007	0.0190
0.8146	0.8013	0.0163
1.0000	0.9858	0.0142

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.0298
0.1519	0.1477	0.0274
0.2944	0.2870	0.0251
0.5097	0.4989	0.0211
0.6078	0.5961	0.0192
0.7017	0.6896	0.0172
0.7038	0.6918	0.0171
0.8620	0.8502	0.0137
1.0000	0.9890	0.0110

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, lized 3 times from absolute ethanol.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.0298
0.1367	0.1329	0.0278
0.2625	0.2557	0.0260
0.2635	0.2567	0.0259
0.4723	0.4618	0.0223
0.5604	0.5489	0.0206
0.6694	0.6569	0.0187
0.8301	0.8169	0.0159
1.0000	0.9870	0.0130

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.0298
0.2044	0.1996	0.0237
0.4105	0.4031	0.0180
0.5112	0.5032	0.0156
0.6135	0.6053	0.0134
0.8046	0.7966	0.0100
1.0000	0.9929	0.0071

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and S.A. Tucker

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.0298
0.1970	0.1915	0.0278
0.3882	0.3785	0.0250
0.4961	0.4844	0.0235
0.5987	0.5852	0.0225
0.7905	0.7752	0.0194
1.0000	0.9841	0.0159

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 372 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.

(3) Gold Label, 99+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

J. Chem. Soc., Faraday Trans. 1990, *86*, 2197-2201.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0085
0.0928	0.0913	0.0162
0.1745	0.1703	0.0243
0.2383	0.2307	0.0317
0.4437	0.4170	0.0602
0.5420	0.5023	0.0733
0.6579	0.6001	0.0879
0.8223	0.7365	0.1044
0.9093	0.8107	0.1084
1.0000	0.8903	0.1097

[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 372 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.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

J. Chem. Soc., Faraday Trans. 1990, *86*, 2197-2201.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0110
0.1019	0.0999	0.0199
0.1946	0.1886	0.0306
0.2541	0.2449	0.0361
0.4668	0.4360	0.0660
0.5695	0.5233	0.0811
0.6673	0.6053	0.0929
0.8323	0.7425	0.1079
1.0000	0.8903	0.1097

[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 372 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.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

J. Chem. Soc., Faraday Trans. 1990, *86*, 2197-2201.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 26.0$ °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0141
0.1130	0.1104	0.0233
0.2119	0.2047	0.0338
0.2735	0.2621	0.0415
0.4930	0.4593	0.0683
0.5937	0.5460	0.0803
0.6867	0.6234	0.0922
0.8519	0.7604	0.1074
1.0000	0.8903	0.1097

[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 372 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.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]	Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I. *J. Chem. Soc., Faraday Trans.* 1990, *86*, 2197-2201.
VARIABLES:	**PREPARED BY:**
T/K = 299, Solvent composition	W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0110
0.0792	0.0776	0.0200
0.1475	0.1433	0.0283
0.1952	0.1883	0.0351
0.3914	0.3674	0.0613
0.4909	0.4549	0.0734
0.5860	0.5360	0.0854
0.7949	0.7142	0.1015
1.0000	0.8903	0.1097

[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 372 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.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

J. Chem. Soc., Faraday Trans. 1990, *86*, 2197-2201.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0130
0.0955	0.0933	0.0233
0.1782	0.1724	0.0328
0.2270	0.2182	0.0389
0.4328	0.4042	0.0661
0.5356	0.4940	0.0777
0.6323	0.5765	0.0882
0.7915	0.7104	0.1025
1.0000	0.8903	0.1097

[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 372 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.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

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

J. Chem. Soc., Faraday Trans. 1990, *86*, 2197-2201.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.0071
0.1163	0.1147	0.0136
0.2129	0.2083	0.0214
0.2737	0.2661	0.0277
0.4940	0.4671	0.0545
0.6464	0.5971	0.0763
0.6898	0.6324	0.0832
0.8535	0.7654	0.1032
1.0000	0.8903	0.1097

[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 372 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.

(3) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA.

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) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

(3) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.0284
0.136	0.131	0.0395
0.296	0.281	0.0513
0.486	0.456	0.0609
0.596	0.558	0.0635
0.716	0.669	0.0656
1.000	0.943	0.0567

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not specified, was recrystallized several times from toluene and ethanol to give a melting point temperature of 150.5-150.9 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

(3) Commercial sample, purity and source not specified, was dehydrated and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.00288
0.111	0.110	0.00584
0.250	0.247	0.0117
0.428	0.419	0.0221
0.667	0.641	0.0385
0.819	0.778	0.0495
1.000	0.943	0.0567

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not specified, was recrystallized several times from toluene and ethanol to give a melting point temperature of 150.5-150.9 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

(3) Commerical sample, purity and source not specified, was dehydrated and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_2: ± 0.001 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 20.0 °C

$x_2^{(s),b}$	x_2	x_1
0.000	0.000	0.0873
0.177	0.161	0.0884
0.364	0.333	0.0858
0.563	0.518	0.0798
0.774	0.719	0.0715
1.000	0.943	0.0567

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

[b] computed by compiler.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities were calculated from the weight of the solid residue which remained after the solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not specified, was recrystallized several times from toluene and ethanol to give a melting point temperature of 150.5-150.9 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

(3) Purity not specified, Urxovy Zavody, was treated with potassium permanganate, dried over potassium hydroxide and then distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.

x_2: ± 0.001 (compiler).

x_1: ± 3 % (relative error; compiler).

THIANTHRENE SOLUBILITIES IN BINARY SOLVENT MIXTURES

I. Alkane + Alkane (including cycloalkanes)

n-hexane + cyclohexane
n-heptane + cyclohexane
n-octane + cyclohexane
methylcyclohexane + cyclohexane
cyclooctane + cyclohexane
2,2,4-trimethylpentane + cyclohexane

II. Alkane + Aromatic Hydrocarbon

None

III. Alkane + Ester

None

IV. Alkane + Ether

None

V. Alkane + Chloroalkane

None

VI. Ether + Chloroalkane

None

VII. Miscellaneous

None

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

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

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

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker, and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00587
0.1754	0.1744	0.00543
0.3094	0.3078	0.00505
0.4494	0.4473	0.00464
0.5538	0.5514	0.00432
0.7567	0.7538	0.00380
0.8677	0.8647	0.00351
1.0000	0.9968	0.00320

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 255 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.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

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

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

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00587
0.1593	0.1584	0.00550
0.3263	0.3246	0.00508
0.4260	0.4239	0.00485
0.5284	0.5260	0.00455
0.7478	0.7448	0.00400
0.8658	0.8626	0.00375
1.0000	0.9965	0.00346

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 255 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.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.
Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00587
0.1444	0.1436	0.00552
0.3019	0.3003	0.00517
0.4010	0.3990	0.00498
0.5006	0.4982	0.00478
0.6683	0.6653	0.00447
0.7228	0.7196	0.00439
0.8528	0.8493	0.00416
1.0000	0.9961	0.00392

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 255 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absoute ethanol.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

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

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

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00587
0.1789	0.1778	0.00591
0.3552	0.3531	0.00601
0.4599	0.4571	0.00610
0.5625	0.5590	0.00616
0.7633	0.7585	0.00623
0.8816	0.8761	0.00626
1.0000	0.9937	0.00631

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

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

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

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00587
0.1705	0.1693	0.00701
0.3522	0.3493	0.00815
0.4506	0.4466	0.00881
0.5564	0.5511	0.00950
0.6318	0.6255	0.00994
0.7568	0.7486	0.01080
0.8455	0.8359	0.01133
1.0000	0.9877	0.01232

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

AUXILIARY INFORMATION

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(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

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

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

ORIGINAL MEASUREMENTS:

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

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr., P.R. Naidu, S.A. Tucker and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.00587
0.1472	0.1464	0.00516
0.3035	0.3021	0.00452
0.3973	0.3956	0.00420
0.4961	0.4942	0.00391
0.6314	0.6292	0.00353
0.7157	0.7133	0.00332
0.8528	0.8502	0.00301
1.0000	0.9973	0.00273

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 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 255 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.

(3) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

SYSTEM INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. All page below refer to compiled tables.

REGISTRY NUMBER INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. All page numbers given below refer to compiled tables

AUTHOR INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. All page numbers below refer to compiled tables.

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