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SOLUBILITY DATA SERIES

Volume 58

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

SOLUBILITY DATA SERIES

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Volume Editor

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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 18column 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 nu

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 dm³ for molar; etc. Usually, only one type of value (e.g., mass per cent) is found in the original paper, and the compiler has added the other type of value (e.g., mole per cent) from computer calculations based on 1989 atomic weights (2). Temperatures are expressed as $t/^{\circ}$ C, $t/^{\circ}$ 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):

$$x_1 = n_1 / \sum_{s=1}^{c} n_s$$
 [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 v_{i+} cations and v_{i-} anions, with $v_i = v_{i+} + v_{i-}$ 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:

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

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

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

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

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

$$x_{1} = \frac{v_{2}x_{01}}{v_{2}-(v_{2}-1)x_{2}} \quad x_{2} = \frac{x_{2}}{v_{2}-(v_{2}-1)x_{2}}$$
[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):

$$w_1 = g_1 / \sum_{s=1}^{c} g_s$$
 [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, $x_{s,1}$:

$$x_{s,1} = m_1 / \sum_{s=1}^{c'} m_s = x_1 / \sum_{s=1}^{c'} x_s$$
^[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, $x_{v,1}$:

$$x_{\nu,1} = x_1 / \sum_{s=1}^{p} x_s$$
 [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 :

$$n_1 = n_1 / n_2 M_2$$

roı

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), $m_1^{(3)}$:

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

SI base units: mol kg⁻¹. Here, the average molar mass of the solvent is

$$M = x_{v,2}M_2 + (1 - x_{v,2})M_3$$
^[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 :

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

$$\rho_1 = g_1 / V = c_1 M_1 / V$$
 [13]

SI base units: kg m⁻³.

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

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

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

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

$$I_m = \frac{1}{2} \sum_i m_i z_i^2, \quad I_c = \frac{1}{2} \sum_i c_i z_i^2$$
 [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_- ,

$$I_m = |z_{+}z_{-}|vm_i, I_c = |z_{+}z_{-}|vc_i$$
 [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 :

$$\rho = g/V = \sum_{s=1}^{c} \rho_s$$
[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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January, 1994

m_i c_i x_i w_i $x_i =$ x_i $1 + \frac{1}{m_t M_c} + \sum_{j \neq i}^{c-1} \frac{m_j}{m_i}$ c-1 $1 + \frac{M_i}{M_c}$ $1 + \frac{1}{M_c} \left(\frac{\rho}{c_i} - M_i \right)$ c-1 'M_c $\frac{w_j}{w_j}$ $w_i =$ $c_i M_i$ wi $1 + \frac{1}{m_i M_i} \left(1 + \sum_{j \neq i}^{c-1} m_j M_j \right)$ $1 + \frac{M_c}{M_c}$ ρ c-1 M. $m_i =$ m_i c-1 c-1 $\frac{1}{c_{i}}$ $\sum_{j \neq i} c_j$ -М, М $c_i =$ $\frac{\rho w_i}{M_i}$ c_i c-1 *c*-1 1 'M_j +*M*_i М,+М *i*≠i

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

 ρ - density of solution; M_1 - molar masses of i. For relations for 2-component systems, set summations to 0.

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PREFACE

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

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

Critical evaluation of published solubility data was performed only if four or more independent sources of experimental data could be found for the particular solutesolvent system under consideration. In the case of isothermal solubility data, where only a single temperature was studied, the published mole fraction solubilities were arithmetically averaged, and the mean and corresponding standard deviation are reported. If experimental solubilities were given at several temperatures, then the critical evaluation involved a linear least squares regression of the natural logarithm of mole fraction solubility versus the reciprocal of absolute temperature, in accordance with accepted thermodynamic practices. The mathematical equation for the

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least squares line and Ln x_1 versus 1/T graph are included in the volume. For a few systems, there was sufficient experimental data to permit construction of the binary phase diagram.

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

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

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

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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 , <u>etc.</u>, (2) amount concentration

$$c_i = [i] = n_i / V$$
 SI base units: mol dm⁻³ [1]

(3) mole fraction

φ.

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

or (4) volume fraction

$$= n_1 V_1 / (n_1 V_1 + n_2 V_2 + n_3 V_3 + \dots)$$
^[3]

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

$$\phi_1 = n_1 V_{m,1} / (n_1 V_{m,1} + n_2 V_{m,2} + n_3 V_{m,3} + \dots)$$
^[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 \underline{i} divided by the mass of the solvent

 $m_i = n_i/n_s M_s$ SI base unit: mol kg⁻¹ [5] where M_s is the molar mass of the solvent.

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

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

- (a) The breaking of solute-solute interactions in the crystalline lattice;
- (b) the breaking of solvent-solvent interactions, often referred to as cavity formation;
- (c) the formation of solute-solvent interactions; and
- (d) the perturbation of solvent-solvent interactions in the immediate vicinity of the solute, as in solvent structuring.

Each of these four contributions may be further divided into specific chemical (complexation) and nonspecific physical (simple dispersion) interactions. To

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

The thermodynamic criterion governing solute solubility (component 1) and solidliquid equilibrium is

 $a_1 = a_1^*$

[6]

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or

$$a_1 = \gamma_1 x_1 a_1^{\circ}$$
 [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, $a_1^*(1)$, 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_{uo} .

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

Step I:Solute 1 (solid, T)Solute 1 (solid, T_{MP})Step II:Solute 1 (solid, T_{MP})Solute 1 (liquid, T_{MP})Step III:Solute 1 (liquid, T_{MP})Solute 1 (liquid, T)with the overall process being

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

 $\Delta G = RT \ln a_1(s) = \Delta G_1 + \Delta G_{11} + \Delta G_{111}$

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

$$\ln a_{1}(s) = \ln (\gamma_{1}x_{1}) = -\Delta H^{fus} (T_{MP} - T)/R T T_{MP} + \Delta C_{p} (T_{MP} - T)/RT - (\Delta C_{p}/R) \ln (T_{MP}/T)$$
[9]

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

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

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

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

^a Melting point temperatures and enthalpy of fusion data for all polycylic aromatic compounds, except for phthalazine, quinazoline and quinoxaline, were taken from published compilations by Acree (9,10). Experimental data for the three diazanaphthalenes was from a calorimetric study by Sabbah and Pemenzi (62). not listed in the table it is possible to estimate ΔH^{fus} from simple geometric considerations and/or group contribution parameters. Enthalpy and entropy are both state functions, and only the initial and final states, *i.e.*, the crystal and the melt, need to be defined. At the molecular level, the two states differ in their relative degree of geometric order. Intermolecular distance, spacial orientation and packing arrangement in the crystalline state are defined within a much narrower range than in the liquid melt.

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

- (a) Translational melting representing the change from the highly ordered arrangement of the molecular gravitational centers in the crystal to the more randomized, expanded arrangement in the liquid; and
- (b) Rotational melting resulting from the change in ordered arrangement of the crystalline molecule's major axis to a randomly oriented arrangement in the liquid.

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

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

[11]

 $\Delta s^{fus} = \Delta s^{trans} + \Delta s^{rot}$

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

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

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

 $\Delta S^{fus} = \sum n_i C_i G_i + \sum n_j C_j G_j + \sum n_k C_K G_k$ [12] For cyclic hydrocarbons

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

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

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

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

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approximately 7 %.

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

- (a) For a given solid-solvent system, the solubility increases with increasing temperature. The rate of increase is approximately proportional to the enthalpy of fusion and, to a first approximation, does not depend upon the melting point temperature.
- (b) For a given solvent and at a fixed temperature, if two solids have a similar entropy of fusion then the solid with the lower melting temperature has the higher solubility. Similarly, if two solids have about the same melting temperature then the one with the lower enthalpy of fusion has the higher solubility.

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

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

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

[16]

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

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

Chiou and Manes (15) compared experimental solubilities of 11 crystalline nonpolar polycyclic aromatic compounds and their derivatives in glycerol trioleate ($v_{m,s} = 966$ cm³ mol⁻¹) to predictions based upon eqns. [9] and [17]. The authors' calculations revealed that the observed mole fraction solubilities are considerably higher than the predictions of eqn. [9] (with $\Delta C_p = 0$); the predictions in some instances being low by as much as 100 percent. In comparison, the observed volume fraction solubilities, ϕ_1 , were comparable to or only slightly lower than the predictions of eqn. [17] (again with $\Delta C_p = 0$). The magnitude of the deviations from Raoult's law is well beyond the uncertainty of the observed solubilities. Since the solubility data can be explained by the Flory-Huggins model and since there is no convincing evidence to indicate strong specific solute-solvent interactions, the observed negative deviations from Raoult's law appears to be an artifact of the model caused by large molecular size disparity. The solubility measurements of Chiou and Manes, combined with an earlier study on glycerol trioleate/water partition coefficients (16), suggest that the Flory-Huggins model should be considered in systems having molar volume ratios of 4 or more.

SCATCHARD-HILDEBRAND SOLUBILITY PARAMETER THEORY

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

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

RT ln $(a_1(s)/x_1) = V_{m,1} (1 - \phi_1)^2 (\delta_1 - \delta_{solvent})^2$ [18] where $\delta_{solvent}$ and δ_1 refer to the solubility parameters of the solvent and supercooled liquid solute, respectively, $V_{m,1}$ is the molar volume of the supercooled liquid solute, x_1 is the saturation mole fraction solubility, and ϕ_1 is the solute's volume fraction solubility calculated using the ideal molar volume approximation (eqn. [4]). For solvent components, the liquid molar volumes and solubility parameters are often tabulated in the literature (for example, see both Hoy (18) and Barton (17)), and when not available, they can be calculated directly from density and vapor pressure measurements on the pure liquid. Molar volumes of supercooled liquid solutes, $V_{m,1}$, on the other hand, are estimated either by group contribution methods or by the experimentally determined apparent partial molar volumes in the solvent of interest. Solubility parameters of the supercooled liquid can be obtained indirectly from solubility measurements or can be estimated by group contribution methods.

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

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

TABLE II. Co	mparison Between	Experimental and	d Predicted Naphthale	ene Solubilities
Solvent	δ2 ^a	v _{m,2} ª	x ₁ (exp) ^b	x ₁ (calc)
Dichloromethan	e 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
Trichlorometha	ne 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
Tetrachloromet	hane 17.49	97.08	0.255	0.275
Cyclohexane	16.75	108.76	0.147	0.242
Methylcyclohex	ane 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 disulfi	de 20.29	60.62	0.283	· 0.311

^a $\delta_2/(10^3 \text{ g/kg}^{1/2} \text{ m}^{-1/2} \text{ s}^{-1}); V_{m,2}/(\text{cm}^3 \text{ mol}^{-1}).$ ^b Experimental solubilites were determined by Chang (63).

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

TABLE III. Comparison Between Experimental and Predicted Biphenyl Solubilities

^a $\delta_2/(10^3 \text{ g/kg}^{1/2} \text{ m}^{-1/2} \text{ s}^{-1}); V_{m,2}/(\text{cm}^3 \text{ mol}^{-1}).$ ^b Experimental solubilities were determined by Chang (63).

 $\delta_{\text{solvent}} = (\phi_2 \ \delta_2 + \phi_3 \ \delta_3)/(\phi_2 + \phi_3) = \phi_2^{(s)} \ \delta_2 + \phi_3^{(s)} \ \delta_3 \qquad [19]$ as a volume fraction average of the solubility parameters of the two pure solvents, δ_2 and δ_3 . The superscript (s) indicates that the solvent composition is calculated as if the solute were not present.

The popularity of the solubility parameter approach arises because it relates the solubility of a solute in a given solvent, either pure or mixed, to the bulk properties of the pure components. Whereas this particular application of the solubility parameter theory has certain practical advantages in that it requires only a minimal number of experimental observations, a more flexible expression for binary solvent systems can be derived by replacing the individual δ_1 values with the measured solubilities in the pure solvents and the measured thermodynamic excess properties of the solvent mixture.

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

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

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

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

 $(G_1^{E})_i^{\circ} = (1 - \phi_1)^{-2} RT \ln (a_1(s)/x_1) = V_{m,1} (\delta_i - \delta_1)^2$ i = 2,3 [22] The small subscripts i = 2 and i = 3 are used to distinguish the properties of the solute in a pure solvent from those in the binary solvent system. Similarly, the excess Gibbs energy of the binary solvent mixture can be expressed

$$G_{23}^{E} = (x_2^{(s)} V_{m,2} + x_3^{(s)} V_{m,3}) \phi_2^{(s)} \phi_3^{(s)} (\delta_2 - \delta_3)^2$$
[23]
in terms of solubility parameters.

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

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

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 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.

[24]

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

$$\log x_1 = -\log a_1(s) + (V_{m,1} \phi_{solvent}^2 \cdot 303 \text{ RT}) [\delta_{solvent}^2 + \delta_1^2 - 2 \Sigma A_i \delta_{solvent}^i]$$

$$[25]$$

derived by Martin and co-workers (19-21) reproduces very accurately the solubility

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

MOBILE ORDER THEORY FOR BINARY ALKANE + ALCOHOL SOLVENT MIXTURES

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

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

McCargar and Acree (29-33) compared values for the carbazole-dibutyl ether association constant calculated from experimental carbazole solubilities in ten binary

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

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

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

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

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

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

 $\ln \phi_{A} = \ln a_{A}(s) - 0.5 (1 - V_{m,A}/V_{m,solvent}) \phi_{solvent} + 0.5 \ln [\phi_{A}^{sat} + \phi_{solvent}(V_{A}/V_{solvent})] - \phi_{solvent}^{2} V_{m,A}(\delta_{A}^{*} - \delta_{solvent}^{*})^{2} (RT)^{-1} - r_{s} (V_{m,A}/V_{m,solvent}) \phi_{solvent}$ [26]

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

 $r_{\rm S} = (K_{\rm S} \ \phi_{\rm solvent} / V_{\rm m, solvent}) / (1 + K_{\rm S} \ \phi_{\rm solvent} / V_{\rm m, solvent})$ with a numerical value of $K_{\rm S} = 5,000 \ {\rm cm}^3 \ {\rm mol}^{-1}$ used for monofunctional alcohols.

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

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

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

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

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

^c Numerical value was calculated using the measured anthracene mole fractions solubility in n-hexane, n-heptane and n-octane, in accordance with eqn. [26]. Pirson (51) or by making approximations based upon known values for similar compounds or homomorphic hydrocarbons.

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

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

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

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

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

$$- (V_{m,A}/V_{m,C}) (K_C \phi_C^0^2/V_{m,C}) / (1 + K_C \phi_C^0/V_{m,C}) = V_{m,A} [\phi_B^{(s)} (\delta_A^i - \delta_B^i)^2 + \phi_C^{(s)} (\delta_A^i - \delta_C^i)^2 - \phi_B^{(s)} \phi_C^{(s)} (\delta_B^i - \delta_C^i)^2]$$

$$[28]$$

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

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

and

$$RT \{ \ln [a_A(s)/(\phi_A)_C] - 0.5(1 - V_{m,A}/V_{m,C}) + 0.5 \ln (V_{m,A}/V_{m,C}) - (V_{m,A} K_C/V_{m,C}^2)/(1 + K_C/V_{m,C}) \} = V_{m,A} (\delta_A^* - \delta_C^*)^2$$
[30]

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

$$\ln \phi_{A} = \phi_{B}^{(s)} \ln (\phi_{A})_{B} + \phi_{C}^{(s)} \ln (\phi_{A})_{C} - 0.5 \left[\ln (x_{B}^{(s)}V_{m,B} + x_{C}^{(s)}V_{m,C}) - \phi_{B}^{(s)} \ln V_{m,B} - \phi_{C}^{(s)} \ln V_{m,C} \right] + \left(V_{m,A} K_{C} \phi_{C}^{(s)} / V_{C}^{2} \right) \left(1 + K_{C} / V_{m,C} \right)^{-1} - \left[V_{m,A} K_{C} \phi_{C}^{(s)2} / V_{m,C}^{2} \right] x \\ \left(1 + \phi_{C}^{(s)} K_{C} / V_{m,C} \right)^{-1} + V_{A} \phi_{B}^{(s)} \phi_{C}^{(s)} \left(\delta_{B}^{*} - \delta_{C}^{*} \right)^{2} \left(RT \right)^{-1}$$
[31]

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

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

critically evaluate the measured solubility data for possible outliers.

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

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

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

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

^a Deviation (%) = (100/N) Σ | ln [x_A(cal)/x_A(exp)].

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

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

MOBILE ORDER THEORY FOR BINARY ALCOHOL + ALCOHOL SOLVENT MIXTURES

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

$$\gamma_{B_{2}} = 1/[1 + K_{B} \phi_{B}/V_{m,B} + K_{BC} \phi_{C}/V_{m,C}]$$
ad

[32]

and

$$Y_{C:} = 1/[1 + K_{CB} \phi_{B}/V_{m,B} + K_{C} \phi_{C}/V_{m,C}]$$
(33)

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

$$G = n_{A} \mu_{A}^{*} + n_{B} \mu_{B}^{*} + n_{C} \mu_{C}^{*} + n_{B} RT \ln \gamma_{B:} + n_{C} RT \ln \gamma_{C:} + 0.5 RT \{n_{A} \ln \phi_{A} + n_{B} \ln \phi_{B} + n_{C} \ln \phi_{C} + n_{A} \ln \phi_{A} + n_{B} \ln \phi_{B} + n_{C} \ln x_{C} \} + (n_{A} \nabla_{m,A} + n_{B} \nabla_{m,B} + n_{C} \nabla_{m,C}) [\phi_{A} \phi_{B} (\delta_{A}^{*} - \delta_{B}^{*})^{2} + \phi_{A} \phi_{C} (\delta_{A}^{*} - \delta_{C}^{*})^{2} + \phi_{B} \phi_{C} (\delta_{B}^{*} - \delta_{C}^{*})^{2}]$$
[34]

and saturation solubility of a sparingly soluble solute

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

 $= (V_{m,A}/V_{m,B}) RT \phi_B^{(s)} (\phi_B^{(s)} (K_B/V_{m,B}) + \phi_C^{(s)} (K_{BC}/V_{m,C})]/[1 + \phi_B^{(s)} (K_B/V_{m,B})$
 $+ \phi_C^{(s)} (K_{BC}/V_{m,C})] = (V_{m,A}/V_{m,C}) RT \phi_C^{(s)} [\phi_B^{(s)} (K_{CB}/V_{m,B}) + \phi_C^{(s)} (K_C/V_{m,C})] +$
 $[1 + \phi_B^{(s)} (K_{CB}/V_{m,B}) + \phi_C^{(s)} (K_C/V_{m,C})]\} = V_{m,A} [\phi_B^{(s)} (\delta_A^* - \delta_B^*)^2 + \phi_C^{(s)} (\delta_A^* - \delta_C^*)^2$
 $- \phi_B^{(s)} \phi_C^{(s)} (\delta_B^* - \delta_C^*)^2]$
[35]

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

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

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

and

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

- $(V_{m,A} K_C/V_{m,C}^2)/(1 + K_C/V_{m,C}) = V_{m,A} (\delta_A^* - \delta_C^*)^2$ [37]

where $(\phi_A^{sat})_B$ and $(\phi_A^{sat})_C$ denote the solubilities in the two pure solvents. After

removal of the $(\delta_A^i - \delta_B^i)^2$ and $(\delta_A^i - \delta_C^i)^2$ terms, one obtains a relatively simple mathematical expression for the solubility in a binary solvent mixture

$$\ln \phi_{A} = \phi_{B}^{(s)} \ln (\phi_{A})_{B} + \phi_{C}^{(s)} \ln (\phi_{A})_{C} - 0.5 [\ln (x_{B}^{(s)}V_{m,B} + x_{C}^{(s)}V_{m,C}) - \phi_{B}^{(s)} \ln V_{m,B} - \phi_{C}^{(s)} \ln V_{m,C}] - (V_{m,A}/V_{m,B}) \phi_{B}^{(s)} [\phi_{B}^{(s)} (K_{B}/V_{m,B}) + \phi_{C}^{(s)} (K_{BC}/V_{m,C})] + [1 + \phi_{B}^{(s)} (K_{B}/V_{m,B}) + \phi_{C}^{(s)} (K_{BC}/V_{m,C})] + (V_{m,A} K_{B} \phi_{B}^{(s)}/V_{m,B}^{2}) (1 + K_{B}/V_{m,B})^{-1} - (V_{m,A}/V_{m,C}) \phi_{C}^{(s)} [\phi_{B}^{(s)} (K_{CB}/V_{m,B}) + \phi_{C}^{(s)} (K_{C}/V_{m,C})]/[1 + \phi_{B}^{(s)} (K_{CB}/V_{m,B}) + \phi_{C}^{(s)} (K_{C}/V_{m,C})] + (V_{m,A} K_{C} \phi_{C}^{(s)}/V_{m,C}^{2}) (1 + K_{C}/V_{m,C})^{-1} + V_{m,A} \phi_{B}^{(s)} \phi_{C}^{(s)} (\delta_{B}^{*} - \delta_{C}^{*})^{2} (RT)^{-1}$$
[38]

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

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

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

INDLE VI.	Summarized Comparison Between Experimental Anthracene Solubilities				
	and Predicted Values Based Upon Equa	tion [37] Derived From Mobile			
	Order Theory for Two Hydrogen-Bondin	g Alcohol Cosolvents			
Solvent (B) + Solvent (C)	% Dev.ª			
1-Butanol	+ 1-Propanol	- 1.0			
2-Butanol	+ 1-Propanol	0.5			
2-Propanol	+ 1-Propanol	1.5			
1-Octanol	+ 1-Propanol	- 2.9			
1-Butanol	+ 2-Propanol	- 1.9			
2-Butanol	+ 2-Propanol	0.3			
1-Octanol	+ 2-Butanol	- 4.1			
AVERAGE AB	SOLUTE DEVIATION	1.7			

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

MATHEMATICAL REPRESENTATION OF SOLUBILITY DATA IN BINARY SOLVENTS

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

 $(Z^{E}_{ABC})^{exp} - (Z^{E}_{ABC})^{calc} = x_{A} x_{B} x_{C} Q_{ABC}$ [39] with Q-functions of varying complexity. For most systems encountered, the experimental data can be adequately represented by a power series expansion

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

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

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

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

$$\ln x_{A} = x_{B}^{(s)} \ln (x_{A})_{B} + x_{C}^{(s)} \ln (x_{A})_{C} + x_{B}^{(s)} x_{C}^{(s)} \Sigma S_{i} (x_{B}^{(s)} - x_{C}^{(s)})^{i}$$
[41]

or Modified Wilson equation

$$\ln (a_{A}(s)/x_{A}) \approx 1 - x_{B}^{(s)} \{1 - \ln [a_{A}(s)/(x_{A})_{B}]\}/(x_{B}^{(s)} + x_{C}^{(s)} \Lambda_{BC}^{adj}) - x_{C}^{(s)} \{1 - \ln [a_{A}(s)/(x_{A})_{C}]\}/(x_{B}^{(s)} \Lambda_{CB}^{adj} + x_{C}^{(s)})$$

$$[42]$$

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

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

Solvent (R) + Solvent (C)	A adj,a	s nev.b
Solvent (b) + Solvent (c)	л ₁ ,	* DEV.
· Tutulaulakana + 0.0 Asteleothulnontano	1 463	0.1
t-Butylcyclonexane + 2,2,4-crimecnyipencane	1.455	0.1
······································	0.301	0.5
n-Hexane + 1-propanol	1.360	0.5
	1.440	
n-Heptane + 1-propanol	1.410	0.7
	1.580	~ ~
n-Octane + 1-propanol	1.240	0.6
<u>.</u>	1.880	
Cyclohexane + 1-propanol	1.300	1.6
	1.600	
Methylcyclohexane + 1-propanol	1.344	1.4
	1.667	- -
2,2,4-Trimethylpentane + 1-propanol	1.100	0.6
	1.500	
t-Butylcyclohexane + 1-propanol	1.225	1.0
	2.321	
n-Hexane + 2-propanol	1.409	0.7
	1.605	
n-Heptane + 2-propanol	0.962	0.6
	2.085	
n-Octane + 2-propanol	0.913	0.3
	2.365	
Cyclohexane + 2-propanol	1.657	0.5
• -	1.701	
Methylcyclohexane + 2-propanol	1.689	0.6
	1.801	
2,2,4-Trimethylpentane + 2-propanol	0.956	0.3
	1.797	
t-Butylcyclohexane + 2-propanol	1.378	1.4
	2.557	
n-Hexane + 1-butanol	1.690	0.4
	1.088	
n-Heptane + 1-butanol	1.476	0.5
	1.291	
n=Octane + 1=butanol	1.460	0.5
	1.500	
Cvclohexane + 1-butanol	2.377	0.5
	1.010	
Mothylevelohovano + 1-butanol	2 387	0.9
Welligteyetonexane · I Securit	1 080	0.5
2 2 A-meimothulmontano + 1-hutanol	2 600	1 9
2/2/4-IIIMethyipentane + I-Datanoz	2.000	1.0
- Putul laborana + 1-butanal	U.000 1 EDE	
C-BACATCACIOUEXQUE + I-DACQUOI	1.525	0.7
· ··	1.007	
n-Hexane + 2-Dutanol	1.477	0.5
	1.481	_
n-Heptane + 2-butanol	1.109	0.3
- • · · •	1.849	
n-Octane + 2-butanol	0.949	0.4
	2.205	

TABLE VII. (Continued)		
Cyclohexane + 2-butanol	2.157 1.345	0.5
Methylcyclohexane + 2-butanol	1.885	0.6
2,2,4-Trimethylpentane + 2-butanol	1.593	0.4
	1.633	
t-Butylcyclohexane + 2-butanol	1.325	0.5
n-Hexane + 1-octanol	2.501	0.6
	0.601	
n-Heptane + 1-octanol	2.201	0.3
n=Octane + l=octanol	1.901	0.2
	0.801	
Cyclohexane + 1-octanol	4.733	0.4
	0.213	0.2
Methylcyclohexane + 1-octanol	0.102	0.2
2.2.4-Trimethylpentage + 1-octagol	2.009	0.3
	0.493	
t-Butylcyclohexane + 1-octanol	3.097	0.3
	0.577	
n-Hexane + 2-methyl-l-propanol	1.557	0.6
	1.417	0 F
n-Heptane + 2-methyl-1-propanol	1.205	0.5
n-Ostano + 2-motbul-1-nyonanol	1.141	0.5
n-occane + 2-methyl-1-propanol	1.969	
Cyclohexane + 2-methy1-1-propanol	2.197	0.6
	1.249	
Methylcyclohexane + 2-methyl-1-propanol	1.961	0.9
	1.501	0.0
2,2,4-Trimethylpentane + 2-methyl-1-propanol	1.525	0.9
t=Butyloycloberane + 2-methyl=l=propanol	1.345	0.5
	2.017	
n-Hexane + 3-methy1-1-butanol	1.709	0.3
	1.149	
n-Heptane + 3-methyl-1-butanol	1.437	0.3
	1.341	0.2
n-Octane + 3-methyl-1-butanol	1.529	0.2
Cycloberane + 3-methyl-1-bytanol	2.449	0.3
Cyclonexane + J-mechyl-1-butanol	0.977	
Methylcyclohexane + 3-methyl-1-butanol	2.453	0.4
	1.061	
2,2,4-Trimethylpentane + 3-methyl-1-butanol	1.449	0.2
	1.121	0.4
t-Butylcyclohexane + 3-methyl-l-butanol	1.561	0.4
-Butanol + lenropanol	1.293	0.2
r promioi + t-broballor	0.857	
2-Propanol + 1-propanol	0.953	0.5
	1.073	

TABLE VII. (Continued)		
2-Butanol + 1-propanol	1.000	0.3
	1.000	
1-Octanol + 1-propanol	0.453	0.4
	2.213	
1-Butanol + 2-propanol	1.169	0.5
	0.989	
2-Butanol + 2-propanol	0.689	0.1
	1.429	
1-Octanol + 2-butanol	0.505	0.6
	1.937	

^a Adjustable parameters for the Modified Wilson equation are ordered as Λ_{BC}^{adj} and then Λ_{CB}^{adj} . ^b & Dev. = (100/N) Σ | ln [x_A (cal)/ x_A (exp)] |.

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

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

TABLE VIII. (Continued)				
n-Octane + 1-butanol	0.933	0.6	0.909	0.4
	- 0.033		- 0.014	
			0.088	
Cyclohexane + 1-butanol	0.810	0.9	0.741	0.5
	0.336		0.345	
			0.223	
Methylcyclohexane + 1-butanol	0.948	1.1	0.850	1.0
	0.282		0.146	
			0.295	
2,2,4-Trimethylpentane + 1-butanol	0.576	0.5	0.536	0.3
	0.121		0.151	
			0.142	
t-Butylcyclohexane + 1-butanol	1.134	1.2	1.039	0.4
	- 0.210		- 0.109	
			0.372	
n-Hexane + 2-butanol	1.165	0.3		
	- 0.081			
n-Heptane + 2-butanol	1.225	0.2		
	- 0.292			
n-Octane + 2-butanol	1.458	1.3		
	- 0.618			
Cyclohexane + 2-butanol	1.260	0.6		
	0.206			
Methylcyclohexane + 2-butanol	1.447	1.2		
	- 0.009			
2,2,4-Trimethylpentane + 2-butanol	1.070	0.8		
	- 0.213			
t-Butylcyclohexane + 2-butanol	1.718	1.7	1.588	0.3
	- 0.612		- 0.493	
			0.497	
n-Hexane + 1-octanol	0.748	1.9	0.607	0.8
	0.488		0.448	
.			0.479	
n-Heptane + 1-octanol	0.488	0.6	0.442	0.3
	0.231		0.229	
0-4			0.159	
n-Octane + 1-octanol	0.330	0.1		
Suclaboratory () astronal	0.135		a	
Cyclonexane + 1-Octanol	0.518	1.6	0.400	0.7
	0.421		0.358	
		. .	0.431	
Methylcyclonexane + 1-octanol	0.574	2.4	0.397	1.0
	0.594		0.549	
	0.460	0.2	0.614	
2,2,4-Trimetnyipentane + 1-octanol	0.469	0.3		
	0.247			
t-butylcyclonexane + 1-octanol	0.428	0.9		
	0.236			
n-nexane + 2-metny1-1-propano1	1.267	1.2	1.177	0.5
	- 0.080		- 0.032	
			0.322	

TABLE VIII. (Continued)					
	1 255			• -	
n-neptane + 2-metny1-1-propanol	- 0 350	1.1	1.284	0.7	
	- 0.350		- 0.301		
n-Ostano - 2-mothul-1-propagol	1 5 40		0.266		
n-occane + 2-mechy1-1-propanor	1.540	1.4	1.422	0.4	
	- 0.570		- 0.464		
Guelebeuene + 2-methul-1-menerel			0.447		
Cyclonexane + 2-methyl-1-propanol	1.214	1.3	1.116	0.3	
	0.148		0.172		
			0.341		
Metnylcyclonexane +	1.462	1.8	1.342	0.6	
2-metny1-1-propanol	- 0.070		0.121		
			0.430		
2,2,4-Trimethylpentane +	1.090	1.5	0.972	0.4	
2-methyl-1-propanol	- 0.221		- 0.100		
			0.462		
t-Butylcyclohexane +	1.688	1.4	1.576	0.1	
2-methyl-1-propanol	- 0.549		- 0.435		
			0.432		
n-Hexane + 3-methyl-1-butanol	0.857	0.8			
	0.186				
n-Heptane + 3-methyl-1-butanol	0.802	0.3			
	0.021				
n-Octane + 3-methyl-1-butanol	1.014	0.6			
	- 0.112				
Cyclohexane + 3-methyl-1-butanol	0.786	1.1			
	0.378				
Methylcyclohexane + 3-methyl-1-butanol	0.880	0.9			
	0.358				
2,2,4-Trimethylpentane +	0.663	0.3			
3-methyl-1-butanol	0.095				
t-Butylcyclohexane +	1.092	0.5			
3-methyl-1-butanol	- 0.087				
1-Butanol + 1-propanol	0.117	0.3			
	0.015				
2-Propanol + 1-propanol	0.068	0.7			
	0.058				
2-Butanol + 1-propanol	0.000	0.3			
	0.000				
1-Octanol + 1-propanol	1.025	1.2			
	- 0.575				
1-Butanol + 2-propanol	0.243	0.6			
	- 0.011				
2-Butanol + 2-propanol	0.097	0.1			
·····	- 0.013				
1-Octanol + 2-butanol	0.871	1.1			
·····	- 0.335				

^a % Dev. = (100/N) Σ | ln [$x_A(cal)/x_A(exp)$] |.

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ACENAPHTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated_Hydrocarbons_(including cycloalkanes)</u>

n-octadecane cyclohexane decahydronaphthalene

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

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

- D. <u>Esters</u>
- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons

trichloromethane tetrachloromethane

G. <u>Alcohols</u>

methanol ethanol 1-propanol 1-octanol

- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>

pyridine thiophene 1,2,3,5-tetranitrobenzene

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Djordjevic, N.M.			
(2) n-Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Thermochim. Acta <u>1991</u> , 177, 109-118.			
VARIABLES:	PREPARED BY:			
Temperature	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
T/K x ₂ x ₁	<i>T/K</i> x ₂ x ₁			
352.4 0.3075 0.6925	363.5 0.0792 0.9208			
356.2 0.2410 0.7590				
359.0 0.1815 0.8185				
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Differential scanning calorimeter.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.			
Mixtures (1.5 - 2.0 mg) of known concen- tration were weighed into aluminum pans, which were then crimped to preclude sample loss during the heating process. Solubil- ities determined by measuring melting	(2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.			
points of binary mixtures using a Perkin- Elmer DSC-2 differential scanning calori- meter and scan rate of 5 K/min.	ESTIMATED ERRORS: T/K : precision \pm 0.3 (compiler). x_1 : \pm 0.0003 (compiler).			

COMPONENTS: (1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]		ORIGINAL I	ORIGINAL MEASUREMENTS: McLaughlin, E.; Zainal, H.A.			
		McLaughl				
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		J. Chem.	J. Chem. Soc. <u>1960</u> , 3854-3857.			
VARIABLES:			PREPARED I	BY:		
Temperature		W.E. Acre	W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	x ₂	<i>*</i> 1	T/K	*2	<i>x</i> 1	
308.7	0.9120	0.0880	330.2	0.7188	0.2812	
323.2	0.7923	0.2077	334.0	0.6547	0.3453	

AUXILIARY INFORMATION					
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer.	(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Purity, source and purification method was not specified.				
noting the temperature at which the last trace of solid solute disappeared.	ESTIMATED ERRORS:				
	T/K: precision \pm 0.1. x_1 : \pm 0.0003 (compiler).				

COMPONENTS:			ORIGINAL M	EASUREMENTS:	
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Cyclohexane; C₆H₁₂; [110-82-7] VARIABLES: Temperature</pre>			Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data <u>1985</u> , 30, 403-409. PREPARED BY: W.E. Acree, Jr.		
EXPERIMENTAL V	ALUES		[
T/K	*2	* 1	T/K	<i>x</i> 2	<i>x</i> 1
303.35	0.9147	0.0853	329.95	0.7016	0.2984
307.35	0.8969	0.1031	334.65	0.6303	0.3697
312.05	0.8726	0.1274	339.85	0.5355	0.4645
316.45	0.8435	0.1565	346.45	0.4008	0.5992
320.95	0.8069	0.1931	354.45	0.2258	0.7742
325.65	0.7579	0.2421			
		AUXILIARY	INFORMATION		
METHOD: APPARA	TUS/PROCEDURI	5	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples		 (1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined. (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received. 			
were rotated while bath temperature slowly increased. Solupility determined by noting the temperature at which the last trace of solid solute disappeared.			ESTIMATED I T/K: prec: x ₁ : ± 0.00	ERRORS: Lsion ± 0.1. 03.	

COMPONENTS:		ORIGINAL ME	ASUREMENTS:		
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]			Coon, J.E.	; Auwaerter	;, J.E.; McLaughlin, E.
(2) Decahydro (91-17-8)	(2) Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8]			e Equilibr.	<u>1989</u> , <i>44</i> , 305-345.
VARIABLES:			PREPARED BY	:	
Temperature			W.E. Acree	, Jr.	
EXPERIMENTAL V	ALUES				
T/K	*2	* 1	T/K	*2	*1
300.7	0.8761	0.1239	327.8	0.6698	0.3302
310.9	0.8127	0.1873	336.0	0.5523	0.4477
318.7	0.7504	0.2496	348.3	0.3403	0.6597
	AUXILIARY				
METHOD: APPARA	METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			 99.2 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution. 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves. 		
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED E $T/K:$ precis $x_1: \pm 0.000$	RRORS: sion <u>+</u> 0.1.)3.		

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COMPONENTS			OPTOTNAL M	ORIGINAL MEASUREMENTS:		
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] (2) Benzene; C ₆ H ₆ ; [71-43-2]			Choi, P.B McLaughli J. Chem.	.; Williams, n, E. Eng. Data <u>1</u>	C.P.; Buehring, K.G.; <u>985</u> , <i>30</i> , 403-409.	
VARIABLES:			PREPARED B	Y:		
Temperature			W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES		I			
т/к	x 2	<i>*</i> 1	T/K	*2	<i>x</i> 1	
306.55	0.7747	0.2253	335.95	0.4899	0.5101	
312.95	0.7276	0.2724	345.75	0.3502	0.6498	
319.85	0.6691	0.3309				
328.05	0.5842	0.4158				
		AUXILIARY	INFORMATION			
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.			(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.			
Mixtures or known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Compa	Label, 99.9+ ny, was used	<pre>%, Aldrich Chemical as received.</pre>	
noting the te trace of soli	mperature at d solute dis	which the last	ESTIMATED	ERRORS :		
		••	$T/K: prec x_1: \pm 0.00$	ision <u>+</u> 0.1. 003.		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Acenaphthene; C ₁₂ H ₁₀ ; [8	3-32-9]	McLaughlin, E.; Zainal, H.A.		
(2) Benzene; C ₆ H ₆ ; [71-43-2	1	J. Chem. Soc. <u>1959</u> , 863-867.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		ł		
<i>т/к x</i> 2		× ₁		
303.8	0.8185	0.1815		
314.6	0.7460	0.2540		
336.4	0.5269	0.4731		
342.6	0.4448	0.5552		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath a thermometer.	nd a precision	(1) Purity not specified, Gesellschaft fur Teerverwertung, passed over an alumina column with benzene eluant.		
Mixtures of known concentration glass ampoules and place temperature to equilibrate. were rotated while bath tem increased. Solubility deter	tions sealed d in constant Samples perature slowly mined by	(2) "AnalaR", was dried over sodium wire and freshly distilled before use.		
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 0.0003 (compiler).		

COMPONENTS:			ORIGINAL I	ORIGINAL MEASUREMENTS:			
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Methylbenzene; C₇H₈; [108-88-3] VARIABLES: Temperature</pre>			Speyers, C.L. Am. J. Sci. <u>1902</u> , 14, 293-302. PREPARED BY:				
							W.E. Acree, Jr.
			EXPERIMENTAL	VALUES			
T/K	*2	<i>x</i> 1	T/K	x 2	x 1		
273.2	0.9212	0.0788	314.8	0.7071	0.2929		
283.5	0.8924	0.1076	334.7	0.5492	0.4508		
297.3	0.8347	0.1653					
		AUXILIARY	(INFORMATION	- <u>-</u>			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF N	ATERIALS:		
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was with- drawn through a coarse filter and anal- yzed by specific gravity. Author noted that evaporation to dryness and weighter		(1) Purit talli point (2) Purit tille	y not given, zed from alc temperature y not given, d before use	Kahlbaum, was recrys- ohol to a melting of 93.5 °C. Kahlbaum, was dis-			
the residue was subject to too much decomposition.		ESTIMATED T/K: prec x,: ± 8 %	ERRORS: cision <u>+</u> 0.1. {relative example	rror, compiler).			

COMPONENTS :			ORIGINAL M	EASUREMENTS	:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]			Coon, J.E	; Auwaerte	r, J.E.; McLaughlin, E.
(2) 1,2,3,4-7 C ₁₀ H ₁₂ ; [1	etrahydronap 19-64-2]	hthalene;	Fluid Pha	se Equilibr	. <u>1989</u> , <i>44</i> , 305-345.
VARIABLES:			PREPARED B	Y:	
Temperature			W.E. Acre	e, Jr.	
EXPERIMENTAL V	ALUES				
T/K	x2	x 1	T/K	*2	×1
308.1	0.7479	0.2521	343.7	0.3825	0.6175
312.6	0.7151	0.2849	351.9	0.2539	0.7461
322.2	0.6359	0.3641			
331.9	0.5305	0.4695			
		AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.			(1) 99.2 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was passed over an activated alumina column and		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last			<pre>then recrystallized from solution. (2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.</pre>		
			ESTIMATED I	ERRORS :	·····
trace of solid solute disappeared.		<i>T/K</i> : prec: <i>x</i> ,: <u>+</u> 0.00	ision <u>+</u> 0.1. 003.		

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ;	[83-32-9]	Kravchenko, V.M.; Pastukhova, I.S.
<pre>(2) 1,2-Dimethylbenzene; [95-47-6]</pre>	с ₈ н ₁₀ ;	Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		•
T/K	x2	×1
247.2	1.000	0.000
246.7	0.978	0.022
246.2	0.956	0.044
245.4	0.945	0.055
253.3	0.935	0.065
261.0	0.917	0.083
271.2	0.886	0.114
287.3	0.821	0.179
302.2	0.739	0.261
313.8	0.653	0.347
324.7	0.564	0.436
332.2	0.488	0.512
342.7	0.362	0.638
351.7	0.249	0.751
359.6	0.136	0.864
368.3	0.000	1.000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:
Phase diagram was determi thermal analysis method (detail in V.M. Kravchenko	ned using a described in , J. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.
U.S.S.R. <u>1939</u> , 13, 133), supplemented by visual observations.		(2) Purity and chemical source were not specified in paper, was distilled before use.
		ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).
<u> </u>		

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Acenaphthene; C.,H.,; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S. Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.		
(2) 1,2,4,5-Tetramethylbenzene; C ₁₀ H ₁₄ ; [95-93-2]			
VARIABLES:	PREPARED BY:		
Temperature	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
т/к x ₂	<i>x</i> ₁		
352.2 1.000	0.000		
347.9 0.918	0.082		
344.3 0.856	0.146		
338.2 0.769	0.231		
332.1 0.689	0.311		
323.6 0.577	0.423		
324.6 0.562	0.438		
325.7 0.553	0.447		
328.2 0.525	0.475		
331.6 0.487	0.513		
338.9 0.410	0.590		
347.4 0.303	0.697		
354.5 0.207	0.793		
363.7 0.072	0.928		
368.3 0.000	1.000		
AUXILIAN	RY INFORMATION		
ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. V.S. B. 1939, 13 Januarota hermana	(1) Purity and chemical source were not specified in paper, was recrystallized before use.		
visual observations.	(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
	ESTIMATED ERRORS:		
	T/K: precision \pm 0.2 (Compiler). x ₁ : \pm 0.002 (Compiler).		

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S.
(2) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.
VARIABLES :	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
<i>т/к ×</i> 2	×1
353.2 1.000	0.000
343.3 0.849	0.151
334.1 0.718	0.282
329.2 0.654	0.346
325.0 0.604	0.396
323.2 0.583	0.417
327.0 0.541	0.459
335.7 0.450	0.550
344.7 0.344	0.656
351.3 0.257	0.743
361.8 0.107	0.893
368.3 0.000	1.000
AUXILIARY METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. <u>1939</u> , 13, 133), supplemented by visual observations.	 Purity and chemical source were not specified in paper, was recrystallized before use. Purity and chemical source were not specified in paper, was recrystallized before use. ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x₁: ± 0.002 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H	1 ₁₀ ; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S.
(2) 2-Methylnaphthaler [91-57-6]	ne; C _{11^H10} ;	Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
T/K	x2	<i>×</i> 1
307.3	1.000	0.000
300.2	0.901	0.099
297.2	0.860	0.140
292.7	0.807	0.193
290.9	0.788	0.212
293.0	0.773	0.227
301.9	0.724	0.276
309.0	0.681	0.319
318.7	0.615	0.385
328.7	0.524	0.476
337.0	0.435	0.565
345.9	0.320	0.680
353.5	0.216	0.784
358.4	0.148	0.852
368.3	0.000	1.000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:
Phase diagram was deter thermal analysis method detail in V.M. Kravchen U.S.S.R. 1939, 13, 133	mined using a l (described in uko, J. Phys. Chem.), supplemented by	 Purity and chemical source were not specified in paper, was recrystallized before use.
visual observations.	,,	(2) Purity and chemical source were not specified in paper, was distilled before use.
		ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x ₁ : \pm 0.002 (Compiler).

<pre>(2) 2,6-Dimethylnaphthalene [581-42-0]</pre>	; C ₁₂ H ₁₂ ;	Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	*2	×1		
383.2	1.000	0.000		
374.5	0.846	0.154		
366.9	0.728	0.272		
360.2	0.626	0.374		
349.0	0.504	0.496		
344.4	0.440	0.560		
339.7	0.402	0.598		
342.9	0.365	0.635		
348.2	0.294	0.706		
356.1	0.183	0.817		
363.5	0.076	0.924		
368.3	0.000	1.000		
		•		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Phase diagram was determined thermal analysis method (des detail in V.M. Kravchenko, J N.S. B. 1939, 12, 133), su	l using a cribed in 7. Phys. Chem. upplemented by	(1) Purity and chemical source were not specified in paper, was recrystallized before use.		
visual observations.		(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
		ESTIMATED ERRORS:		
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).		

ORIGINAL MEASUREMENTS:

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

COMPONENTS:

(1) Acenaphthene; C₁₂H₁₀; [83-32-9]

	ODIGINAL MEACIDENTING.			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S.			
(2) 2,7-Dimethylnaphthalene; C ₁₂ H ₁₂ ; [582-16-1]	Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.			
VARIABLES:	PREPARED BY:			
Temperature	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
T/K ×2	×1			
370.2 1.000	0.000			
364.4 0.904	0.096			
361.0 0.858	0.142			
354.4 0.756	0.244			
347.3 0.650	0.350			
340.2 0.555	0.445			
335.3 0.496	0.504			
333.9 0.469	0.531			
334.8 0.449	0.551			
338.7 0.420	0.580			
344.3 0.348	0.652			
352.9 0.214	0.786			
360.7 0.100	0.900			
368.3 0.000	1.000			
AUXILIARY	INFORMATION			
ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.			
v.s.s.k. <u>1939</u> , 13, 133), supplemented by visual observations.	(2) Purity and chemical source were not specified in paper, was recrystallized before use.			
	ESTIMATED ERRORS:			
	T/K: precision \pm 0.2 (Compiler). $x_1: \pm$ 0.002 (Compiler).			

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COMPONENTS:		ORIGINAL MEASUREMENTS:			
 (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Anthracene; C₁₄H₁₀; [120-12-7] 		Kravchenko, V.M.; Pastukhova, I.S. Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	x2	x ₁			
489.7	1.000	0.000			
477.2	0.822	0.178			
466.2	0.706	0.294			
456.2	0.590	0.410			
443.2	0.484	0.516			
434.2	0.397	0.603			
418.2	0.294	0.706			
402.5	0.216	0.784			
387.5	0.156	0.844			
368.2	0.104	0.896			
361.2	0.086	0.914			
362.7	0.071	0.929			
364.4	0.051	0.949			
369 3	0.000	1,000			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:			
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. <u>1939</u> , 13, 133), supplemented by visual observations.		 (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use. ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). 			
		x ₁ : ± 0.002 (Compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S.
(2) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
T/K ×2	x 1
372.5 1.000	0.000
357.4 0.801	0.199
347.7 0.707	0.293
338.7 0.614	0.386
329.0 0.508	0.492
334.5 0.459	0.541
339.1 0.401	0.599
346.7 0.314	0.686
355.0 0.204	0.796
362.0 0.099	0.901
368.3 0.000	1.000
CUA	CILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. C U.S.S.R. <u>1939</u> , 13, 133), supplemente visual observations.	 (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use.
	ESTIMATED ERRORS: T/K : precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

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COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S. Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.			
(2) Fluorene; C ₁₆ H ₁₀ ; [86-73-7]				
VARIABLES:	PREPARED BY:			
Temperature	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
т/К ×2	x ₁			
387.2 1.000	0.000			
379.6 0.889	0.111			
367.9 0.746	0.254			
356.0 0.619	0.381			
348.1 0.528	0.472			
339.3 0.438	0.562			
337.8 0.418	0.582			
340.9 0.382	0.618			
348.2 0.293	0.707			
355.6 0.194	0.806			
361.7 0.103	0.897			
368.3 0.000	1.000			
AUXILIAF	Y INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. <u>1939</u> , 13, 133), supplemented by visual observations.	 (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use. ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x₁: ± 0.002 (Compiler). 			

(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] (2) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] VARIABLES: P Temperature EXPERIMENTAL VALUES	<pre>Kravchenko, V.M.; Pastukhova, I.S. Proc. Acad. Sci. U.S.S.R., Sect. Chem. <u>1956</u>, 111, 667-669 (English translation) PREPARED BY: W.E. Acree, Jr. x₁ 0.000 0.147</pre>
(2) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] VARIABLES: P Temperature EXPERIMENTAL VALUES	Proc. Acad. Sci. U.S.S.R., Sect. Chem. <u>1956</u> , 111, 667-669 (English translation) PREPARED BY: W.E. Acree, Jr. x ₁ 0.000 0.147
VARIABLES: P Temperature EXPERIMENTAL VALUES	PREPARED BY: W.E. Acree, Jr. x1 0.000 0.147
Temperature	W.E. Acree, Jr. x ₁ 0.000
EXPERIMENTAL VALUES	x ₁ 0.000
	x ₁ 0.000
T/K x ₂	0.000
528.2 1.000	0.147
513.2 0.853	0.147
500.2 0.722	0.278
477.8 0.613	0.387
471.5 0.501	0.499
457.0 0.404	0.596
437.4 0.296	0.704
416.2 0.204	0.796
378.5 0.101	0.899
364.2 0.072	0.928
366.4 0.034	0.966
368.2 0.000	1.000
AUXILIARY INI	FORMATION
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. <u>1939</u> , 13, 133), supplemented by visual observations.	 Purity and chemical source were not specified in paper, was recrystallized before use. Purity and chemical source were not specified in paper, was recrystallized before use. STIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x₁: ± 0.002 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83	-32-9]	Kravchenko, V.M.; Pastukhova, I.S.
(2) Fluoranthene; C ₁₆ H ₁₀ ; [20	6-44-0]	J. Gen. Chem. U.S.S.R. <u>1959</u> , 29, 29-34. (English translation)
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
Т/К	×2	x 1
383.2	1.000	0.000
368.8	0.815	0.185
363.4	0.752	0.248
350.7	0.606	0.394
340.8	0.492	0.508
335.0	0.438	0.562
335.3	0.429	0.571
339.4	0.388	0.612
348.2	0.293	0.707
358.1	0.163	0.837
362.3	0.092	0.908
368.3	0.000	1.000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kraychenko, J. Phys. Chem.		 Purity and chemical source were not specified in paper, was recrystallized before use.
U.S.S.R. <u>1939</u> , <i>13</i> , 133), sur visual observations.	opiemented by	(2) Purity and chemical source were not specified in paper, was recrystallized before use.
	-	ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:			
 (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Trichloromethane; CHCl₃; [67-66-3] 		Speyers, C.L. Am. J. Sci. <u>1902</u> , 14, 293-302.			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES		1			
T/K	x2	×1			
273.0	0.8728	0.1272			
284.4	0.8346	0.1654			
325.9 0.5783		0.4219			
	AUXILIARY	' INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was with- drawn through a coarse filter and anal- yzed by specific gravity. Author noted that evaporation to dryness and weighing		 Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C. Purity unknown, several sources listed, washed with water, sulfuric acid, dried over calcium chloride and distilled. 			
the residue was subject decomposition.	to too much	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 8 % (relative error, compiler).			

COMPONENTS:		ORIGINAL MEASUREMENTS:				
 (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Tetrachloromethane; CCl₄; [56-23-5] 			McLaughlin, E.; Zainal, H.A. <i>J. Chem</i> . Soc. <u>1960</u> , 2485-2488.			
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL V	LUES		•			
т/К	*2	x1	T/K	x2	×1	
303.2	0.8195	0.1805	325.2	0.6415	0.3585	
314.6	0.7373	0.2627				
318.6	0.7013	0.2987				
		AUXILIARY	INFORMATION			
METHOD: APPARAT	US/PROCEDURE	3	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		 Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant. AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use. 				
noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED I T/K: prec: $x_1: \pm 0.00$	ERRORS: ision <u>+</u> 0.1. 003 (compiler	:).		

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] (2) Methanol; CH ₄ O; [67-56-1]			Speyers, C.L. Am. J. Sci. <u>1902</u> , 14, 293-302.			
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL V	/ALUES		ļ			
T/K	x2	×1	T/K	×2	<i>x</i> ₁	
273.2	0.9961	G 0039	319.2	0.9845	0.0155	
285.6	0.9962	0.0038	335.5	0.9754	0.0246	
303.9	0.9927	0.0073				
		AUXILIARY	INFORMATION	1	· · · · · · · · · · · · · · · · · · ·	
METHOD: APPAR	TUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	ATERIALS:	
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30		(1) Purity not given, Kahlbaum, was recrys- tallized from alcohol to a melting point temperature of 93.5 °C.				
minutes. Saturated solution was with- drawn through a coarse filter and anal- yzed by specific gravity. Author noted that evaporation to dryness and weighing		(2) Marked "Acetonfrei", from Kahlbaum, dried over calcium oxide and distilled before use.				
the residue w	vas subject to	o too much	ESTIMATED	ERRORS :		
			T/K: prec x ₁ : ± 8 %	ision <u>+</u> 0.1. (relative en	rror, compiler).	

COMPONENTS:			ORIGINAL M	ORIGINAL MEASUREMENTS:		
 (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Ethanol; C₂H₆O; [64-17-5] 		Speyers, (Speyers, C.L. Am. J. Sci. <u>1902</u> , 14, 293-302.			
		Am. J. Sc:				
VARIABLES:			PREPARED BY	:		
Temperature			W.E. Acree	e, Jr.		
EXPERIMENTAL V	VALUES		<u>.</u>			
T/K	x 2	<i>x</i> 1	T/K	*2	<i>*</i> 1	
273.2	0.9943	0.0057	323.0	0.9614	0.0386	
283.2	0.9916	0.0084	344.8	0.8706	0.1294	
303.5	0.9830	0.0170				
		AUXIL	LARY INFORMATION			
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	

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

- (1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.
- (2) Marked absolute, from Eimer and Amend and Chas. Cooper and Co., dried over calcium oxide and distilled before use.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x₁: \pm 8 % (relative error, compiler).

COMPONENTS			ORIGINAL MEASUREMENTS:				
COMPONENTIS							
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) 1-Propanol; C₃H₈O; [71-23-8]</pre>			Speyers, C.L.				
			Am. J. S.	Am. J. Sci. <u>1902</u> , 14, 293-302.			
VARIABLES:		<u></u>	PREPARED BY:				
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL	VALUES						
T/K	x 2	x 1	T/K	<i>x</i> 2	x 1		
273.2	0.9912	0.0088	323.5	0.9563	0.0437		
283.7	0.9903	0.0097	346.6	0.801	0.199		
304.3	0.9812	0.0188					
		AUXILIARY	INFORMATION	1			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:				
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was with- drawn through a coarse filter and anal-			 Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C. Purity not given, Kahlbaum, was dried over calcium oxide and distilled 				
yzed by specific gravity. Author noted that evaporation to dryness and weighing			befor	e use.			
the residue	was subject to	o too much	ESTIMATED	ERRORS :			
	decomposition.			T/K: precision \pm 0.1. x ₁ : \pm 8 % (relative error, compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. <i>Environ. Sci. Technol.</i> <u>1985</u> , <i>19</i> , 522-529.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C c ₁ /	(mol dm ⁻³)			
25.0 0.2	561			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection. Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 %	 Highest available commercial purity, specific chemical supplier not given, was used as received. 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received. 			
SE30 ultraphase column.	ESTIMATED ERRORS: $T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (relative error; compiler).			

			ORTGINAL MEASUREMENTS:				
COMPONENTS			ORIGINAL MERSOREMENTS:				
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]			Choi, P.B.; McLaughlin, E.				
(2) Pyridine; C ₅ H ₅ N; [110-86-1]			Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-51.				
VARIABLES:			PREPARED B	Y:			
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL V	ALUES						
T/K	*2	<i>x</i> 1	T/K	x ₂	<i>x</i> 1		
306.7	0.7898	0.2102	343.7	0.3890	0.6113		
320.0	0.6834	0.3166					
332.9	0.5408	0.4592					
337.5	0.4809	0.5191					
		AUXILIARY	INFORMATION		•		
METHOD: APPARI	TUS/PROCEDURI	5	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			 (1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined. (2) Gold Label, 99.9+ %, Aldrich Chemical 				
					ab lecelveu.		
noting the te trace of sol	emperature at id solute dis	which the last	ESTIMATED	ERRORS:			
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		T/K: precision ± 0.1. x_1 : ± 0.0003.				

COMPONENTS:			ORIGINAL MEASUREMENTS:			
 (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Thiophene; C₄H₄S; [110-02-1] 			Choi, P.B.; McLaughlin, E. Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-51.			
VARIABLES:			PREPARED F	SY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL V	ALUES					
T/K	x 2	<i>x</i> 1	T/K	*2	x 1	
307.3	0.7416	0.2584	344.8	0.3572	0.6428	
319.6	0.6458	0.3542				
328.4	0.5593	0.4407				
335.7	0.4776	0.5224				
		AUXILIARY	INFORMATION	1		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE ANI	D PURITY OF M	ATERIALS:	
Constant temp thermometer.	perature bath	and a precision	(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.			
noting the te trace of soli	were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			ERRORS: cision <u>+</u> 0.1. 003.		

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COMPONENTS :		ORIGINAL MEASUREMENTS:		
(1) Acenaphthene; C ₁₂ H ₁₀ ;	[83 - 32-9]	Shinomiya, C.		
(2) 1,2,3,5-Tetranitroben C ₆ H ₂ N ₄ O ₈ ; [3698-53-1]	zene;	J. Chem. Soc. Japan <u>1940</u> , 15, 259-270.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
т/к	*2	× ₁		
399.2	1.000	0.000		
388.2	0.802	0.198		
382.2	0.706	0.296		
381.7	0.572	0.428		
383.2	0.470	0.530		
381.2	0.429	0.571		
372.2	0.290	0.710		
362.7	0.235	0.765		
348.2	0.118	0.882		
361.7	0.099	0.901		
369.2	0.000	1.000		
	AUXILIAR	Y INFORMATION		
METHOD: APPARATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:		
No experimental details g	iven in paper.	(1) Purity and chemical source were not specified in paper.		
		(2) Purity and chemical source were not specified in paper.		
		ESTIMATED ERRORS:		
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).		

ACRIDINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane decahydronaphthalene

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene 1,2,3,4-tetrahydronaphthalene

- D. <u>Esters</u>
- E. Ethers
- F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>
- G. Alcohols
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>

pyridine thiophene

J. Binary Solvent Mixtures

COMPONENT'S :			ORIGINAL MEASUREMENTS:			
<pre>(1) Acridine; C₁₃H₉N; [260-94-6] (2) Cyclohexane; C₆H₁₂; [110-82-7]</pre>			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.			
VARIABLES:			PREPARED BY:			
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
т/к	<i>x</i> 2	x 1	T/K	x 2	x 1	
309.3	0.9791	0.0209	353.3	0.7550	0.2450	
320.3	0.9697	0.0303	356.1	0.7029	0.2971	
330.9	0.9508	0.0492				
345.4	0.8931	0.1069				
		AUXILIARY	INFORMATION	ł		
METHOD: APPAR	ATUS/PROCEDUR	2	SOURCE AND PURITY OF MATERIALS:			
Constant temp thermometer.	Constant temperature bath and a precision thermometer.			 (1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %. 		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.			
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
trace of sol:	ia solute dis	appeared.	$T/K:$ precision \pm 0.1. $x_1: \pm$ 0.0003.			

COMPONENTS: (1) Acridine; C ₁₃ H ₉ N; [260-94-6] (2) Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8] VARIABLES:			ORIGINAL MEASUREMENTS:			
			Coon, J.E.; Auwaerter, J.E.; McLaughlin, E Fluid Phase Equilibr. <u>1989</u> , 44, 305-345.			
						PREPARED BY:
			Temperature		W.E. Acree, Jr.	
EXPERIMENTAL	VALUES		1			
т/ К	*2	×1	T/K	<i>x</i> 2	<i>*</i> 1	
306.0	0.9705	0.0295	354.7	0.6791	0.3209	
320.7	0.9537	0.0463	358.1	0.6037	0.3963	
335.0	0.9031	0.0969				
345.7	0.8150	0.1850				
		AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.			 (1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum 			

thermometer.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.
New York, USA, was purified by vacuum sublimation to a purity of 99.87 %.
(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.
ESTIMATED ERRORS:
T/K: precision ± 0.1. x₁: ± 0.0003.

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Acridine; C ₁₃ H ₉ N; [260-94-6]			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.				
(2) Benzene;	(2) Benzene, C ₆ n ₆ , (71-43-2)			J. Solution Chem. <u>1988</u> , 16, 519-534.			
VARIABLES:			PREPARED E	BY:			
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL V	VALUES						
T/K	x ₂	*1	T/K	<i>x</i> 2	×1		
296.3	0.8996	0.1004	330.3	0.7122	0.2878		
304.7	0.8680	0.1320	335.6	0.6559	0.3441		
317.2	0.8002	0.1998					
324.2	0.7587	0.2413					
		AUXILIARY	INFORMATION	4			
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer.			(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the te	emperature at	which the last	ESTIMATED	ERRORS:			
trace or sold	ra sointe dis:	appearea.	T/K: precision ± 0.1. x_1 : ± 0.0003.				

COMPONENTS:			ORIGINAL MEASUREMENTS:			
<pre>(1) Acridine; C₁₃H₉N; [260-94-6] (2) 1,2,3,4-Tetrahydronaphthalene;</pre>			Coon, J.E Fluid Pha	.; Auwaerter ase Equilibr.	;, J.E.; McLaughlin, E. <u>1989</u> , 44, 305-345.	
$C_{10}H_{12};$ [119-64-2]						
VARIABLES:			PREPARED B	Y:	······	
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES		I			
<i>т/</i> к	*2	*1	T/K	×2	*1	
305.2	0.8517	0.1483	331.3	0.6956	0.3044	
306.9	0.8409	0.1591	336.7	0.6537	0.3463	
316.3	0.8023	0.1977				
322.4	0.7608	0.2392				
		AUXILIARY	INFORMATION	r		
METHOD: APPAR	ATUS/PROCEDURI	E	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.			(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was vacuum sublimed to a final purity of 99.87 %.			
in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.			
noting the temperature at which the last			ESTIMATED	ERRORS :	······	
trace of sol	noting the temperature at which the last trace of solid solute disappeared.			T/K: precision ± 0.1. $x_1: \pm 0.0003.$		

COMPONENTS:			ORIGINAL MEASUREMENTS:			
<pre>(1) Acridine; C₁₃H₉N; [260-94-6] (2) Pyridine; C₅H₅N; [110-86-1] VARIABLES:</pre>			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. <i>J. Solution Chem.</i> <u>1988</u> , 16, 519-534.			
			Temperature			W.E. Acre
EXPERIMENTAL V	ALUES					
T/K	*2	×1	T/K	*2	×1	
301.7	0.8385	0.1615	339.1	0.5899	0.4101	
309.3	0.7986	0.2014	339.9	0.5616	0.4384	
322.9	0.7209	0.2791				
328.5	0.6600	0.3400				
		AUXILIARY	INFORMATION	4		
METHOD: APPARS	ATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:			
Constant temp thermometer.	perature bath	and a precision	(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			 (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received. 			
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
Crace of 8011	ra solute dis:	appeared.	T/K: precision ± 0.1. x_1 : ± 0.0003.			

COM	COMPONENTS: (1) Acridine; C ₁₃ H ₉ N; [260-94-6] (2) Thiophene; C ₄ H ₄ S; [110-02-1] VARIABLES: Temperature			ORIGINAL MEASUREMENTS: Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534. PREPARED BY: W.E. Acree, Jr.			
(1 (2							
VAR							
Te							
EXP	ERIMENTAL	VALUES					
	T/K	*2	<i>x</i> 1	T/K	*2	×1	
	302.1	0.8203	0.1797	331.6	0.6497	0.3503	
	304.1	0.8024	0.1976	337.9	0.6115	0.3885	
	314.2	0.7563	0.2437				
	325.0	0.7056	0.2944				
			AUXILIARY	INFORMATION	ſ		
MET	HOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:			
Co th Mi in ter we	Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			 (1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %. (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received. ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 0.0003. 			
1n no tr							

ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

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

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

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

D. <u>Esters</u>

ethyl ethanoate butyl ethanoate dimethyl hexanedioate diethyl hexanedioate dibutyl oxalate

E. Ethers

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

F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>

trichloromethane tetrachloromethane iodoethane 1-chlorobutane 1,4-dichlorobutane trichloroethylene iodobenzene bromobenzene chlorobenzene
```
G. Alcohols
```

```
methanol
1-propanol
2-propanol
1-butanol
2-butanol
2-methyl-1-propanol
3-methyl-1-butanol
1-octanol
phenol
1-hydroxy-2-methylbenzene
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H. Ketones
```

2-propanone 2-butanone

I. <u>Miscellaneous Pure Solvents</u>

```
acetonitrile
carbon disulfide
acetic anhydride
dimethyl sulfoxide
nitrobenzene
aniline
pyridine
quinoline
thiophene
methoxybenzene
1-methyl-2-pyrrolidinone
N,N-dimethylacetamide
N,N-dimethylformamide
tetramethylene sulfone
tributyl phosphate
1,2,3,5-tetranitrobenzene
2,4,6-trinitrophenol
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J. <u>Binary Solvent Mixtures</u>

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

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Acree, W.E., Jr.; Rytting, J.H.		
(2) n-Hexane; C ₆ H ₁₄ ; [110	-54-3]	J. Pharm Sci. <u>1983</u> , 72, 292-296.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	*2	× ₁		
25.0	0.9987	0.001290		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDU	RE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		 Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.		
Concentrations determined spectrophoto- metrically at 356 nm.		ESTIMATED ERRORS:		
		$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.		
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x2 ⁸	x1 ^a		
25.0 0.99853	0.00150		
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.			
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision balance.	 Purity and source not given. Purity and source not given. 		
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliguots of saturatured solu-			
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained	ESTIMATED ERRORS:		
after solvent had evaporated.	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).		

ORIGINAL MEASUREMENTS: COMPONENTS: Acree, W.E., Jr.; Rytting, J.H. (1) Anthracene; C14H10; [120-12-7] (2) n-Heptane; C₇H₁₆; [142-82-5] J. Pharm Sci. 1983, 72, 292-296. PREPARED BY: VARIABLES: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES ¢/°C *x*2 **x**1 0.9984 0.001571 25.0 AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. (2) 99 %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves and distilled shortly before use. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of satcoarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-ESTIMATED ERRORS: metrically at 356 nm. $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Lissi, E.A.; Abuin, E.B.		
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.		
VARIABLES:	PREPARED BY:		
T/K = 293	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C c ₁ /	(mol dm ⁻³)		
20.0 0.0	040		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifu- gation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming	(2) Purity and chemical source not given, purification procedure not specified.		
that the dilute solution behavior extra- polates up to saturation point.	ESTIMATED ERRORS:		
	T/K: <u>+</u> 2. c ₁ : unknown.		

(0)/(D0)/(D)/(D)	ODICINAL MERCIDENENTS .
COMPONENTS:	ORIGINAL MEASUREMIS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7	Acree, W.E., Jr.; Rytting, J.H.
(2) n-Octane; C ₈ H ₁₈ ; [111-65-9]	J. Pharm Sci. <u>1983</u> , 72, 292-296.
VARIABLES:	PREFARED DI:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x ₁
25.0 0.99	0.001850
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calor thermometer, and an ultraviolet, spectrophotometer.	<pre>:imetric (1) Gold Label, 99.9 %, Aldrich Chemical /visible Company, Milwaukee, Wisconsin, USA,</pre>
Excess solute and solvent placed glass bottles and allowed to equifor several days at constant ter Attainment of equilibrium verifi repetitive measurements. Aliquot urated solutions transferred the coarse filter into tared volume flasks, weighed and diluted with	<pre>i in amber iilibrate mperature. led by cough a tric n methanol.</pre> (2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectr metrically at 356 nm.	cophoto- ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	McCargar, J.W.; Acree, W.E., Jr.		
(2) n-Hexadecane; $C_{16}H_{34}$; [544-76-3]	J. Pharm. Sci. <u>1987</u> , 76, 572-574.		
VARIABLES: PF	REPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	×1		
25.0 0.9962	0.00380		
AUXILIARY INF	FORMATION		
METHOD: APPARATUS/PROCEDURE SC	OURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-	(2) 99 %, Aldrich Chemical Company, was used as received.		
chloromethane. Concentrations determined spectrophotometrically at 356 nm.	STIMATED ERRORS:		
2	T/K: \pm 0.05. x ₁ : \pm 1 % (relative error).		

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COMPONENTS		OPTOTNAL MEA	SUBENENTS		
COMPONENTS:					
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Djordjevic,	N.M.		
(2) n-Octadeo	cane; C ₁₈ H ₃₈ ;	[593-45-3]	Thermochim.	Acta <u>1991</u>	, 177, 109-118.
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree,	Jr.		
EXPERIMENTAL V	VALUES		8		
T/K	*2	×1	T/K	*2	<i>x</i> 1
466.5	0.4423	0.5577	477.5	0.2000	0.8000
468.0	0.4091	0.5909	478.5	0.1857	0.8143
472.6	0.3226	0.6774	480.8	0.1487	0.8513
477.0	0.2385	0.7615	483.0	0.0989	0.9011
AUXILIARY I			INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND P	URITY OF MA	TERIALS:	
Differential scanning calorimeter.		(1) Gold La Company used as	bel, 99+ %, , Milwaukee received.	Aldrich Chemical , Wisconsin, USA, was	
Mixtures (1.5 - 2.0 mg) of known concen- tration were weighed into aluminum pans, which were then crimped to preclude sample loss during the heating process. Solubil- ities determined by measuring melting points of binary mixtures using a Perkin- Elmer DSC-2 differential scanning calori- meter and scan rate of 5 K/min.		(2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.			
		ESTIMATED ERRORS:			
		T/K: precision \pm 0.3 (compiler). x_1 : \pm 0.0003 (compiler).			

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C₁₄H₁₀; [120-12-7] Acree, W.E., Jr.; Rytting, J.H. (2) Cyclohexane; C₆H₁₂; [110-82-7] J. Pharm Sci. 1983, 72, 292-296. VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C **x**2 x, 25.0 0.9984 0.001574 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. spectrophotometer. (2) 99.5 %, Phillips Petroleum, Bartles-ville, Oklahoma, USA, was stored over molecular sieves and distilled shortly Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by before use. repetitive measurements. Aliquots of sat-urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 356 nm. ESTIMATED ERRORS:

 $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

COMPONENTS:		ORIGINAL N	œasurements:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Coon, J.H McLaughli	E.; Sediawan, In, E.	W.B.; Auwaerter, J.E.;	
(2) Cyclonexa	ine; c ₆ n ₁₂ ; [1	10-82-7]	J. Solution Chem. <u>1988</u> , 16, 519-534.		
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acre	e, Jr.		
EXPERIMENTAL V	VALUES				
T/K	×2	x 1	T/K	x2	x 1
346.8	0.9905	0.0095	391.2	0.9625	0.0375
358.5	0.9857	0.0143	402.4	0.9500	0.0500
366.8	0.9810	0.0190			
378.3	0.9745	0.0255			
		AUXILIARY	INFORMATION	4	
METHOD: APPARATUS/PROCEDURE		SOURCE AND	D PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.		(1) 99.99 Milwa talli	9+ %, Aldrich Aukee, Wiscon Lzed from tol	Chemical Company, sin, USA, was recrys- uene.	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(2) Gold Compa	Label, 99.9+ any, was used	<pre>%, Aldrich Chemical as received.</pre>	
		ESTIMATED	ERRORS:		
		$\begin{array}{c} T/K: \text{ pred}\\ x_1: \pm 0.0 \end{array}$	cision <u>+</u> 0.1. 0003.		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.
VARIABLES:	PREPARED BY:
T/K = 313	W.E. Acree, Jr.
	<u> </u>

EXPERIMENTAL VALUES

t/°C	x2ª	<i>x</i> 1 ^a
40.0	0.9969	0.00306

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

AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliguots of saturatured solu-	(1) Purity and source not given.(2) Purity and source not given.		
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.5 (compiler). x_1 : \pm 5 % (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Tucker, S.A.; Acree, W.E., Jr.		
<pre>(2) Methylcyclohexane; C₇H₁₄; [108-87-2]</pre>	Phys. Chem. Liq. <u>1989</u> , 20, 31-38.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EIPERIMENTAL VALUES			
t/°C x ₂	x 1		
25.0 0.9984	0.00165		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company was stored over mole- cular sieves and distilled shortly before use.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:		
	$T/K: \pm 0.05.$ x ₁ : ± 1 % (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Rytting, J.H.		
(2) Cyclooctane; C ₈ H ₁₆ ; [292-64-8]	J. Pharm Sci. <u>1983</u> , 72, 292-296.		
VARIABLES:	PREPARED BY:		
<i>T</i> /K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	x ₁		
25.0 0.9977	0.002258		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:		
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).		

COMPONENTS :		ORIGINAL MEASUREMENTS:			
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]</pre>		Acree, W.E., Jr.; Rytting, J.H. J. Pharm Sci. <u>1983</u> , 72, 292-296.			
VARIABLES:	· · · · · · · · · · · · · · · · · · ·	PREPARED BY:			
<i>T/</i> K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	x2	×1			
25.0	0.9989	0.001087			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature ba thermometer, and an ult spectrophotometer.	th, calorimetric raviolet/visible	(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.			
Excess solute and solve glass bottles and allow for several days at con Attainment of equilibri repetitive measurements urated solutions transf coarse filter into tare flasks, weighed and dil	nt placed in amber ed to equilibrate stant temperature. um verified by . Aliquots of sat- erred through a d volumetric uted with methanol.	(2) 99+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecu- lar sieves and distilled shortly before use.			
Concentrations determined spectrophoto- metrically at 356 nm.		ESTIMATED ERRORS:			
		$T/K: \pm 0.05.$ x.: ± 1 % (relative error).			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Anderson, B.D.
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C C ₁ /	(mol dm ^{•3})
25.0 0.0	0660
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.

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

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

ESTIMATED ERRORS:

T/K: \pm 0.1 (compiler). c₁: \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.			
(2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1]	J. Chem. Eng. Data <u>1994</u> , 39, 117-118.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂	<i>x</i> 1			
25.0 0.9980	0.001978			
AUXILIARY	INFORMATION			
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.			
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:			
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).			

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		McCargar, J.W.; Acree, W.E., Jr.			
(2) 2,6,10,15,19,23-Hexamethyltetraco- sane (squalane); C ₃₀ H ₆₄ ; [111-01-3]		J. Pharm. Sci. <u>1987</u> , 76, 572-574.			
VARIABLES:		PREPARED BY:			
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	<i>x</i> ₂	x 1			
25.0 0.9953		0.00472			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-		(2) 99 %, Aldrich Chemical Company, was used as received.			
chloromethane. Concentrations determined spectrophotometrically at 356 nm.		ESTIMATED ERRORS:			
		$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).			

r						
COMPONENTS :		ORIGINAL M	EASUREMENTS :			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Coon, J.E	.; Auwaerter	, J.E.; McLaughlin, E.		
<pre>(2) Decahydronaphthalene; C₁₀H₁₈; [91-17-8]</pre>		Fluid Pha	se Equilibr.	<u>1989</u> , <i>44</i> , 305-345.		
VARIABL	ES:			PREPARED B	Y:	
Temperature		W.E. Acre	e, Jr.			
EXPERIM	ENTAL VAL	UES				
T/1	к	x2	<i>*</i> 1	T/K	*2	×1
32	3.6	0.9921	0.0079	362.9	0.9701	0.0299
32	7.1	0.9913	0.0087	385.6	0.9413	0.0587
34:	2.5	0.9849	0.0151			
35	1.0	0.9796	0.0204			
			AUXILIARY	INFORMATION	ſ	
METHOD:	APPARATU	S/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.		(1) 99.99 wauke recei	 Aldrich e, Wisconsin ved. 	Chemical Company, Mil- , USA, was used as		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) 99+ % isome trans	, Aldrich Ch r ratio of 6 , stored ove	emical Company, having 0.6 % cis and 39.4 % r molecular sieves.		
noting the temperature at which the last		ESTIMATED	ERRORS:			
trace of solid solute disappeared.		$T/K: prec x_1: \pm 0.00$	ision <u>+</u> 0.1. 003.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Rytting, J.H.
(2) Benzene; C ₆ H ₆ ; [71-43-2]	J. Pharm Sci. <u>1983</u> , 72, 292-296.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x 1
25.0 0.992	6 0.007418
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calori thermometer, and an ultraviolet/v spectrophotometer.	<pre>metric (1) Gold Label, 99.9 %, Aldrich Chemical isible Company, Milwaukee, Wisconsin, USA, used as received.</pre>
Excess solute and solvent placed glass bottles and allowed to equi for several days at constant temp Attainment of equilibrium verifie repetitive measurements. Aliquots urated solutions transferred thro coarse filter into tared volumetr flasks, weighed and diluted with	<pre>in amber librate erature. d by s of sat- ugh a ic methanol.</pre> (2) Spectroanalyzed, 99.9+ %, Fisher Chem- ical Company, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectro metrically at 356 nm.	photo- ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

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COMPONENTS:		ORIGINAL MEASUREMENTS:			
 (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Benzene; C₆H₆; [71-43-2] 		Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.			
T/K = 293 and 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	*2	x ₁			
20.0	0.9940	0.00595			
25.0	0.9929	0.00711			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, t and a precision balance. Excess solute and solvent pi glass container and allowed for several hours at constar Aliquots of saturated soluti transferred into tared const weighed. Solubilities calcu	thermometer, laced in closed to equilibrate of temperature. Jons were cainers and plated from	 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. 99 %, Commercial sample, source and purification method was not specified. 			
weight of solid residue that after solvent had evaporated	: remained d.	ESTIMATED ERRORS: T/K: precision ± 0.05. x: + 3 % (relative error: compiler).			

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Benzene; C ₆ H ₆ ; [71-43-2] VARIABLES:		ORIGINAL MEASUREMENTS: Somayajulu, G.R.; Palit, S.R. J. Phys. Chem. <u>1954</u> , 58, 417-421.						
						PREPARED BY:		
						Temperature		W.E. Acro
		EXPERIMENTAL	VALUES					
T/K	x2	×1	T/K	×2	×1			
305.2	0.9909	0.00912	320.2	0.9856	0.01437			
310.2	0.9894	0.01059	325.2	0.9830	0.01698			
315.2	0.9875	0.01245	330.2	0.9807	0.01934			
			340.2	0.9744	0.02558			
		AUXILIARY	INFORMATION	4				
METHOD: APPARATUS/PROCEDURE		SOURCE AND	D PURITY OF M	ATERIALS:				
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Repor- ted values computed from variation of mole fraction solubility with temperature.		 Purity not specified, J. T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate. tallized from toluene. AR Grade, thiophene free, source not specified, was dried over calcium chloride and distilled before use 						
		ESTIMATED ERRORS:						
		T/K: precision \pm 0.3. x_1 : \pm 0.00001 (compilier).						

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Benzene; C ₆ H ₆ ; [71-43-2]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.			
VARIABLES:			PREPARED P	BY:	
Temperature		W.E. Acre	ee, Jr.		
EXPERIMENTAL	VALUES		1		
T/K	*2	<i>x</i> 1	T/K	x2	x 1
308.9	0.9899	0.0101	353.9	0.9607	0.0393
330.6	0.9797	0.0203	364.3	0.9501	0.0499
338.2	0.9743	0.0257			
344.6	0.9697	0.0303			
		AUXILIARY	INFORMATION	ſ	
METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(1) 99.99 Milwa talli (2) Gold Compa	+ %, Aldrich ukee, Wiscon zed from tol Label, 99.9+ ny, was used	Chemical Company, sin, USA, was recrys- uene. %, Aldrich Chemical as received.	
		ESTIMATED T/K: prec x ₁ : <u>+</u> 0.00	ERRORS: ision <u>+</u> 0.1. 003.		

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.			
(2) Benzene; C ₆ H ₆ ; [71-43-2]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EIPERIMENTAL VALUES	**************************************			
t/°C x ₂ ^a	x1 ^a			
25.0 0.9926	0.00740			
^a computed by compiler from published so solubilities, which were expressed as we solute per 100 grams of solvent.	olvent compositions and solute eight percent and grams of			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer, and a precision balance.	(1) Purity and source not given.(2) Purity and source not given			
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliquots of saturatured solu-				
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.5 (compiler). x_1 : \pm 5 % (relative error; compiler).			

COMPONENTS: (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Benzene; C₆H₆; [71-43-2]

EVALUATOR:

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Department of Chemistry
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Denton, Texas 76203-5068 (USA)
June, 1994
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CRITICAL EVALUATION:

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

Regressional analysis of the experimental data as Ln x_1 versus 1/T yielded the following mathematical relationship: $\langle \ \ \rangle$

Ln $x_1 = -3200.1 (1/T) + 5.7899$ (r = 0.9987) or 2 for variation of anthracene solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.00713$, and differs by less than 4 % from experimental values of $x_1 = 0.00711$ (4), $x_1 = 0.00748$ (5) and $x_1 = 0.00740$ (6).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

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    Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem.
1988, 16, 519-534.
    Somayajulu, G.R.; Palit, S.R. J. Phys. Chem. 1954, 58, 417-421.
    McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1959, 863-867.
    Smutek, M.; Fris, M.; Fohl, J. Coll. Czech. Chem. Commun. 1967, 32, 931-943.
    Acree, W.E., Jr.; Rytting, J.H. J. Pharm. Sci. 1983, 72, 292-296.
    Mahieu, J. Bull. Soc. Chim. Belgique 1936, 45, 667-677.
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COMPONENTS	,,,,		ORTGINAL	MEASUREMENTS	
COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]			McLaughl.	in, E.; Zaina	1, H.A.
(2) Benzene	; C ₆ H ₆ ; [71-43-	·2]	J. Chem.	<i>s</i> oc. <u>1959</u> ,	863-867.
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acr	ee, Jr.		
EXPERIMENTAL	VALUES				
T/K	*2	<i>x</i> 1	T/K	*2	* 1
309.0	0.9897	0.0103	343.4	0.9685	0.0315
315.6	0.9870	0.0130			
323.8	0.9827	0.0173			
332.8	332.8 0.9775 0.0225				
		AUXILIARY	INFORMATIO	N	
METHOD: APPA	RATUS/PROCEDUR	E	SOURCE AN	D PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.		 Purity, source and purification proce- dure not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(2) "AnalaR", was dried over sodium wire and freshly distilled before use.			
		ESTIMATED	ERRORS:		
		<i>T/K</i> : pred x ₁ : <u>+</u> 0.0	cision <u>+</u> 0.1. 0003 (compile:	r).	

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3] VARIABLES: T/K = 298 EIPERIMENTAL VALUES	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. PREPARED BY: W.E. Acree, Jr.		
t/°c ×2	×1		
25.0 0.9926	0.00736		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).		

COMPONENTS			ORTGINAL D	EASUREMENTS :	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3]		Smutek, M Collectic 32, 931-9	M.; Fris, M.; Dn Czech. Che 943.	Fohl, J. m. Commun. <u>1967</u> ,	
VARIABLES:			PREPARED I	BY:	
T/K = 293, 313 and 333		W.E. Acro	ee, Jr.		
EXPERIMENTAL V	ALUES				
t/°C	*2	<i>*</i> 1	t/°C	x ₂	×1
20.0	0.9935	0.00645	60.0	0.9770	0.0230
40.0	0.9876	0.0124			
		AUXILIARY	INFORMATION	4	·
METHOD: APPARATUS/PROCEDURE		SOURCE AND	D PURITY OF M	ATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from		 (1) 95 % Czech timer to gi (2) 99 %, purii 	initial puri n., was recry s from pyridin lve a final pu , Commercial s fication metho	ty, Urxovy Zavady, stallized several ne and cyclohexane urity of 98.3 %. sample, source and od was not specified.	
weight of solid residue that remained after solvent had evaporated.		ESTIMATED T/K: pred $x_1: \pm 3$ %	ERRORS: cision <u>+</u> 0.05. (relative er	rror; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Tucker, S.A.; Acree, W.E., Jr.	
(2) 1,4-Dimethylbenzene; C ₈ H ₁₀ ; [106-42-3]	Phys. Chem. Liq. <u>1989</u> , 20, 31-38.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	×1	
25.0 0.9927	0.00733	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) HPLC Grade, 99.5+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: ± 0.05 . x ₁ : ± 1 % (relative error).	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Smutek, M.; Fris, M.; Fohl, J.	
(2) 1,4-Dimethylbenzene; C ₈ H ₁₀ ; [106-42-3]	Collection Czech. Chem. Commun., <u>1967</u> , 32, 931-943.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	×1	
25.0 0.9923	0.00770	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. 99 %, Commercial sample, source and purification method was not specified. 	
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).	

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Wheeler, A.S.			
<pre>(2) 4-Isopropyl methylbenzene; C₁₀H₁₄; [99-87-6]</pre>		J. Am. C	hem. Soc. <u>19</u>	20, 42, 1842-1846.	
VARIABLES:			PREPARED	BY:	
Temperature		W.E. Acr	ee, Jr.		
EXPERIMENTAL V	ALUES		<u></u>		
т/к	*2	×1	<i>т/</i> к	*2	x 1
298.2	0.9883	0.0117	373.2	0.9349	0.0651
303.2	0.9872	0.0128			
		AUXILIARY	INFORMATIO	N	
METHOD: APPARATUS/PROCEDURE			SOURCE AND	D PURITY OF M	ATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass containers and allowed to equili-			(1) Purit (2) Purit	ty and source	not given. not given.
brate for several hours at constant temperature, Aliquots of saturatured solu-					
tions transferred into tared containers and weighed. Solubilities calculated from weight of solid residue which remained after solvent had evaporated.		ESTIMATED	ERRORS :		
		T/K: pred x ₁ : ± 5 %	cision <u>+</u> 0.5 (relative en	(compiler). rror; compiler).	

COMPONENTS:	C	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-	7]	Kravchenko, V.M.; Pastukhova, I.S.		
(2) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] VARIABLES:		Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.		
		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES	79 <u>2 </u>			
T/K ×2		x 1		
368.3 1.0	000	0.000		
364.4 0.9	49	0.051		
362.7 0.9	29	0.071		
361.2 0.9	14	0.086		
368.2 0.8	96	0.104		
387.5 0.8	44	0.156		
402.5 0.7	84	0.216		
418.2 0.7	06	0.294		
434.2 0.6	03	0.397		
443.2 0.5	16	0.484		
456.2 0.4	10	0.590		
466.2 0.2	94	0.706		
477.2 0.1	78	0.822		
489.7 0.0	00	1.000		
	AUXILIARY IN	IFORMATION		
METHOD: APPARATUS/PROCEDURE	s	OURCE AND PURITY OF MATERIALS:		
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem.		 Purity and chemical source were not specified in paper, was recrystallized before use. 		
visual observations.		(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
	E	STIMATED ERRORS:		
		T/K: precision \pm 0.2 (Compiler). x ₁ : \pm 0.002 (Compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:
 (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Chrysene; C₁₈H₁₂; [218-01-9] 		Kravchenko, V.M.; Pastukhova, I.S.
		Proc. Acad. Sci. U.S.S.R., Sect. Chem. <u>1956</u> , 111, 667-669 (English translation)
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		1
T/K	×2	×1
528.2	1.000	0.000
519.2	0.896	0.104
509.5	0.788	0.212
499.7	0.693	0.307
490.9	0.603	0.397
480.4	0.496	0.504
470.5	0.402	0.598
466.2	0.365	0.635
467.2	0.303	0.697
469.7	0.260	0.740
473.7	0.202	0.798
481.7	0.103	0.897
489.7	0.000	1.000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Phase diagram was determin thermal analysis method (d detail in V.M. Kravchenko, U.S.S.R. 1939, 12, 133)	ed using a escribed in J. Phys. Chem. supplemented by	(1) Purity and chemical source were not specified in paper, was recrystallized before use.
visual observations.		(2) Purity and chemical source were not specified in paper, was recrystallized before use.
		ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).
L		

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-	-12-7]	Kravchenko, V.M.; Pastukhova, I.S.
(2) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]		J. Gen. Chem. U.S.S.R. <u>1959</u> , 29, 29-34. (English translation)
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
T/K	*2	<i>x</i> ₁
383.2	1.000	0.000
377.8	0.930	0.070
376.5	0.906	0.094
375.0	0.884	0.116
374.2	0.860	0.140
380.2	0.859	0.141
387.3	0.830	0.170
395.7	0.804	0.196
419.9	0.671	0.329
435.2	0.566	0.434
449.4	0.456	0.544
459.7	0.355	0.645
467.4	0.269	0.731
475.1	0.178	0.822
489.7	0.000	1.000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Phase diagram was determined thermal analysis method (des detail in V.M. Kravchenko, J U.S.S.P. 1939, 133), sm	i using a scribed in 7. Phys. Chem.	 Purity and chemical source were not specified in paper, was recrystallized before use.
visual observations.	,pp_001002 27	(2) Purity and chemical source were not specified in paper, was recrystallized before use.
	·	ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS:		ORIGINAL M	EASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Coon, J.E	.; Auwaerter	, J.E.; McLaughlin, E.		
(2) 1,2,3,4-Tetrahydronaphthalene; C ₁₀ H ₁₂ ; [119-64-2]			Fluid Pha	se Equilibr.	<u>1989</u> , <i>44</i> , 305-345.	
VARI	ABLES:			PREPARED B	Y:	
Temperature		W.E. Acre	e, Jr.			
EXPE	RIMENTAL VA	LUES				
	T/K	x2	×1	T/K	*2	x 1
	299.6	0.9900	0.0100	343.4	0.9592	0.0408
	319.5	0.9801	0.0199	346.2	0.9567	0.0433
	327.6	0.9741	0.0259			
	333.0	0.9697	0.0303			
			AUXILIARY	INFORMATION	r	
METH	METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples			(1) 99.99 wauke recei (2) 99.6+ store	 Aldrich Wisconsin ved. Aldrich over molec 	Chemical Company, Mil- , USA, was used as Chemical Company, was ular sieves to remove	
were rotated while bath temperature slowly increased. Solubility determined by			trace water.			
noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED	ERRORS:			
		$T/K: prec x_1: \pm 0.00$	ision <u>+</u> 0.1. 003.			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.		
(2) Ethyl ethanoate; C ₄ H ₈ O ₂ ; [141-78-6]	Phys. Chem. Liq. <u>1991</u> , 24, 31-42.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		

EXPERIMENTAL VALUES

t/°C	*2	x 1
25.0	0.9952	0.00484

AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flags upped and diluted with methanol	(2) 99.5+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.		
(2) Butyl ethanoate; C ₆ H ₁₂ O ₂ ; [123-86-4]	J. Chem. Soc. Faraday Trans. <u>1991</u> , 87, 461-464.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	<i>x</i> 1		
25.0 0.9934	0.00661		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:		
	$T/K: \pm 0.05.$ x,: ± 1 % (relative error).		

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Dimethyl hexanedioate; C ₈ H ₁₄ O ₄ ; [627-93-0] VARIABLES: T/K = 298 EIPERIMENTAL VALUES	ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr. Phys. Chem. Liq. <u>1992</u> , 25, 51-58. PREPARED BY: W.E. Acree, Jr.	
t/°C x ₂	<i>x</i> ₁	
25.0 0.9913	0.00871	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use. 	
metrically at 356 nm.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).	

COMPONENTS	······································	OPTGINAL MEASUDEMENTS.
COMPORENTS		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Acree, W.E., Jr.
(2) Diethyl hexanedioat [141-28-6]	:e; C ₁₀ H ₁₈ O ₄ ;	Phys. Chem. Liq. <u>1991</u> , 24, 31-42.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	x 2	x 1
25.0	0.9897	0.01033
<u> </u>	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.
Concentrations determined spectrophoto- metrically at 356 nm.		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Dibutyl Ovalate: C H.O.:	Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr.	
(2) 515dcy1 0x414ce, 01011802, (2050-60-4)	Phys. Chem. Liq. <u>1992</u> , 25, 51-58.	
VARIABLES:	PREPARED BY:	
<i>T/K</i> = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.9896	0.01043	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1.5 $ (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.	
(2) 1,1-Oxybisethane; C ₄ H ₁₀ O; [60-29-7]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂ ª	x1 ^a	
25.0 0.9965	0.00353	
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer,	(1) Purity and source not given.	
and a precision balance.	(2) Purity and source not given.	
Excess solute and solvent placed in closed glass containers and allowed to equili-		
brate for several hours at constant temperature. Aliguots of saturatured solu-		
tions transferred into tared containers	ESTIMATED EDDODS:	
weight of solid residue which remained after solvent had evaporated.		
	$x_1: \pm 5$ (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Marthandan, M.V.; Acree, W.E., Jr.	
(2) 1,1-Oxybisbutane; C ₈ H ₁₈ O; [142-96-1]	J. Chem. Eng. Data <u>1987</u> , 32, 301-303.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	<i>x</i> 1	
25.0 0.9964	0.003609	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.05. x_1 : \pm 1 % (relative error).	

COMPONENTS:		ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1,1-Oxybisbutane; C₈H₁₈O; [142-96-1]</pre>		McCargar, J.W.; Acree, W.E., Jr. J. Pharm. Sci. <u>1987</u> , 76, 572-574.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C x	2	x 1
25.0 0	.9965	0.00354
	AUXILIARY I	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra- chloromethane. Concentrations determined spectrophotometrically at 356 nm.		(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Anderson, B.D.	
(2) 1,1-Oxybisbutane; C ₈ H ₁₈ O; [142-96-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C c ₁ /0	(mol dm ⁻³)	
25.0 0.0	210	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature.	 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received. 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received. 	
Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). c ₁ : \pm 3 % (relative error; compiler).	
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) Tetrahydrofuran; C ₄ H ₈ O; [109-99-9]	Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.991 0.00	09
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS :	OPTOINAL MEASUREMENTS.	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Tetrahydropyran; C₅H₁₀O; [142-68-7] </pre>	Bissell, M.; Chittick, C.E.; Acree, W.E., Jr. Fluid Phase Equilibr. <u>1988</u> , 41, 187-194.	
VARIABLES:	PREPARED BY:	
<i>T/K</i> = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.9898	0.01024	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in ambeu glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol	(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company was stored over mole- cular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).	

	OBICINAL MEACIDEMENTS.
COMPONENTS	URIGINAL MEASUREMENIS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-17-7] (2) 1,4-Dioxane; C,H₀O₂; [123-91-1]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44.
402	(English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.9904 0.00	096
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).
4	

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) 1,4-Dioxane; C ₄ H ₈ O ₂ ; [123-91-1] VARIABLES: T/K = 298	ORIGINAL MEASUREMENTS: Procyk, A.D.; Bissell, M.; Street, K.W., Jr.; Acree, W.E., Jr. J. Pharm. Sci. <u>1987</u> , 76, 621-626. PREPARED BY: W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	×1	
25.0 0.9916	0.008381	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) HPLC Grade, 99.8 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).	

COMPONENTS: ORIGINAL MEASUREMENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1,4-Dioxane; C₄H₈O₂; [123-91-1] Environ. Sci. Technol. <u>1990</u>, 24, 639-646. PREPARED BY: VARIABLES: W.E. Acree, Jr. T/K = 296EXPERIMENTAL VALUES $c_1/(\text{mol dm}^{-3})$ t/°C 23.0 0.0756 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, centrifuge, (1) Purity not given, commercial sample of thermometer, and an HPLC equipped with uv absorption and fluorescence detection. unspecified source, was used as received. Excess solute and solvent were placed in glass vials and allowed to equilibrate (2) Purity and chemical source not given, purification procedure not specified. with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

ESTIMATED ERRORS:

 $c_1: \pm 5$ % (relative error; compiler).

 $T/K: \pm 1.$

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Smutek, M.; Fris, M.; Fohl, J.
<pre>(2) Trichloromethane; CHCl₃; [67-66-3]</pre>	;	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	*2	×1
25.0	0.9895	0.0105
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	·····	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from		 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. 99 %, Commercial sample, source and purification method was not specified.
after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).	

T			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.		
<pre>(2) Trichloromethane; CHCl₃; [67-66-3]</pre>	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂ ª	x ₁ ª		
25.0 0.9893	0.0107		
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.			
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision balance.	(1) Purity and source not given.(2) Purity and source not given.		
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Alignots of saturatured solu-			
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained	ESTIMATED ERRORS:		
after solvent had evaporated.	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).		

COMPOMENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Tucker, S.A.; Acree, W.E., Jr.
<pre>(2) Tetrachloromethane; CC1₄; [56-23-5]</pre>	Phys. Chem. Liq. <u>1989</u> , 19, 73-79.
VARIABLES:	PREPARED BY:
<i>T</i> /K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	×1
25.0 0.9954	0.00464
AUXILIA	RY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).
METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol Concentrations determined spectrophoto- metrically at 356 nm.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before us ESTIMATED ERRORS: T/K: ± 0.05. x₁: ± 1 % (relative error).</pre>

COMPONENTS:		ORIGINAL	MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Smutek, M.; Fris, M.; Fohl, J.			
<pre>(2) Tetrachloromethane; CCl₄; [56-23-5]</pre>		Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.			
VARIABLES:			PREPARED BY:		
T/K = 293, 298, 313 and 333		W.E. Acr	ee, Jr.		
EXPERIMENTAL VALUES					
t/°C	*2	x 1	t/ºC	*2	x 1
20.0	0.9959	0.00411	40.0	0.9916	0.00836
25.0	0.9952	0.00483	60.0	0.9844	0.0156
		AUXILIARY	INFORMATIO	N	
METHOD: APPARATUS/PROCEDURE		SOURCE AN	D PURITY OF M	ATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.		(1) 95 % Czec time to g (2) 99 % puri	initial puri h., was recry s from pyridi ive a final p , Commercial ; fication meth	ty, Urxovy Zavady, stallized several ne and cyclohexane urity of 98.3 %. sample, source and od was not specified.	
		ESTIMATED T/K: pre	ERRORS: cision <u>+</u> 0.05 (relative end	rror; compiler).	

COMPONENTS :		ORIGINAL N	ORIGINAL MEASUREMENTS:				
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Somayaju	Somayajulu, G.R.; Palit, S.R.				
(2) Iodoethane; C ₂ H ₅ I; [74-88-4] 75-03-6			J. Phys.	J. Phys. Chem. <u>1954</u> , 58, 417-421.			
VARIABLES:	i		PREPARED I	PREPARED BY:			
Temperature		W.E. Acro	ee, Jr.				
EXPERIMENTAL	VALUES		!				
T/K	×2	x 1	T/K	*2	×1		
310.2	0.9881	0.01189	340.2	0.9713	0.02867		
320.2	0.9839	0.01612					
330.2	0.9783	0.02175					
		AUXILIA	ARY INFORMATIO	N			
METHOD: APPARATUS/PROCEDURE			SOURCE AN	D PURITY OF M	IATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by visu- noting the temperature at which the last		(1) Purit was ethan tall (2) Purit author Y and o	ty not specif recrystallize nol and ethyl ized from tol ty not specif ors, dried ov distilled bef	ied, J. T. Bake d several times ethanoate. uene. ied, prepared b er calcium chlor ore use.	r, USA, from Y ride		
noting the temperature at Which the last trace of solid solute disappeared. Repor- ted values computed from variation of mole fraction solubility with temperature			$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $	cision ± 0.3.	er)		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.
(2) 1-Chlorobutane; C ₄ H ₉ Cl; [109-69-3]	J. Solution Chem. <u>1991</u> , 20, 307-318.
VARIABLES:	PREPARED BY:
<i>T</i> /K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x 1
25.0 0.9941	0.00586
;	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorim thermometer, and an ultraviolet/vi- spectrophotometer.	etric (1) Gold Label, 99.9+ %, Aldrich Chemical sible Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in glass bottles and allowed to equil for several days at constant tempe Attainment of equilibrium verified repetitive measurements. Aliquots of urated solutions transferred throw coarse filter into tared volumetrin flasks, weighed and diluted with mu	<pre>1 amber lbrate rature. by of sat- gh a c ethanol.</pre> (2) HPLC Grade, 99.5+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectrop metrically at 356 nm.	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1.5 $ % (relative error).

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) 1,4-Dichlorobutane; C ₄ H ₈ Cl ₂ ; [110-56-5] VARIABLES:		ORIGINAL MEASUREMENTS:		
		Acree, W.E., Jr.; Zvaigzne, A.I.		
		Phys. Chem. Liq. <u>1991</u> , 23, 225-237.		
		PREPARED BY:		
<i>T/</i> K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	*2	x ₁		
25.0	0.9895	0.01053		
	AUXIL	IARY INFORMATION		

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	(2) puriss, 99+ %, Fluka Chemical Corpora- tion, Ronkonkoma, New York, USA, was stored over molecular sieves and dis- tilled shortly before use.
	ESTIMATED ERRORS:
	$x_1: \pm 1.5$ % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:		
 (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Trichloroethylene; C₂HCl₃; [79-01-6] 	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. <i>Environ. Sci. Technol.</i> <u>1990</u> , 24, 639-646.		
VARTABLES:	PREPARED BY:		
T/K = 296	W.E. Acree, Jr.		
EIPERIMENTAL VALUES			
t/°C c ₁ /(mol dm ⁻³)		
23.0 0.0	0.0705		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.		
fluorescence or uv detection.	ESTIMATED ERRORS:		
	T/K: \pm 1. c_1 : \pm 5% (relative error; compiler).		

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Iodobenzene; C ₆ H ₅ I; [591-50-4] VARIABLES:		ORIGINAL MEASUREMENTS:				
		Somayajulu, G.R.; Palit, S.R. J. Phys. Chem. <u>1954</u> , 58, 417-421.				
						PREPARED BY:
		Temperature		W.E. Acree, Jr.		
EXPERIMENTAL	VALUES	·····				
T/K	*2	×1	T/K	*2	<i>*</i> 1	
305.2	0.9854	0.01462	320.2	0.9766	0.02344	
310.2	0.9827	0.01728				
315.2	0.9799	0.02014				
		AUXILIARY	INFORMATION	N		
METHOD: APPARATUS/PROCEDURE		SOURCE AND	D PURITY OF M	IATERIALS:		
Constant temperature bath and a precision thermometer.		(1) Purit was n ethan	ty not specif recrystallize nol and ethyl	ied, J. T. Baker, d several times f ethanoate.	USA, rom	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Repor- ted values computed from variation of mole fraction solubility with temperature.		tallized from toluene.(2) Purity not specified, Columbia Organic Chemicals, was distilled before use.			anic e.	
		ESTIMATED T/K: pred $x_1: \pm 0.0$	ERRORS: cision ± 0.3. 0001 (compil	ier).		

COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.			
(2) Bromobenzene; C ₆ H ₅ Br; [108-86-1]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂ *	<i>x</i> 1 ^a			
25.0 0.9881	0.0119			
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.				
AUXILIARY	INFORMATION			
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer,	(1) Purity and source not given.			
and a precision balance.	(2) Purity and source not given.			
Excess solute and solvent placed in closed				
brate for several hours at constant				
tions transferred into tared containers				
and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS:			
	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.			
<pre>(2) Chlorobenzene; C₆H₅Cl; [108-90-7]</pre>	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂ ^a	x1 ^a			
25.0 0.9897	0.0103			
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.				
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer, and a precision balance.	 Purity and source not given. Purity and source not given. 			
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliguots of saturatured solu-				
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained	ESTIMATED ERRORS:			
after solvent had evaporated.	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).			

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COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	<pre>Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.</pre>		
(2) Chlorobenzene; $C_{\delta}H_5C1$; [108-90-7]	Environ. Sci. Technol. <u>1990</u> , 24, 639-646.		
VARIABLES:	PREPARED BY:		
T/K = 296	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C c ₁ /	(mol dm ⁻³)		
23.0 0.0	0.0628		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	 Purity not given, commercial sample of unspecified source, was used as received. 		
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.		
fluorescence or uv detection.	ESTIMATED ERRORS:		
	$T/K: \pm 1.$ $c_1: \pm 5$ (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Smutek, M.; Fris, M.; Fohl, J.	
(2) Methanol; CH ₄ O; [67-56-1]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.	
VARIABLES:	PREPARED BY:	
T/K = 293	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
20.0 0.9998	0.000202	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.	 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. 99 %, Commercial sample, source and purification method was not specified. 	
	ESTIMATED ERRORS: T/K : precision \pm 0.05.	
	$x_1: \pm 3$ % (relative error; compiler).	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.	
(2) Methanol; CH ₄ O; [67-56-1]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x2 ⁸	x1 ^a	
25.0 0.9997	0.000252	
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.		
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer,	(1) Purity and source not given.	
and a precision balance.	(2) Purity and source not given.	
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliguots of saturatured solu-		
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).	

ORIGINAL MEASUREMENTS: COMPONENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. (1) Anthracene; C14H10; [120-12-7] (2) Methanol; CH40; [67-56-1] Environ. Sci. Technol. 1990, 24, 639-646. PREPARED BY: VARIABLES: W.E. Acree, Jr. T/K = 296EXPERIMENTAL VALUES t/°C $c_1/(\text{mol dm}^{-3})$ 0.00477 23.0 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.
 Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.
 (1) Purity not given, commercial sample of unspecified source, was used as received.
 (2) Purity and chemical source not given, purification procedure not specified.
 (2) Purity and chemical source not given, purification procedure not specified.
 (2) Purity and chemical source not given, purification procedure not specified.
 (2) Furity and chemical source not given, purification procedure not specified.
 (3) RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.
 ESTIMATED ERRORS:
 T/K: ± 1. C₁: ± 5% (relative error; compiler).

Components:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.	
(2) 1-Propanol; C ₃ H ₈ O; [71-23-8]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂ ª	<i>x</i> ₁ ^a	
25.0 0.9996	0.000371	
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.		
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance.	(1) Purity and source not given.(2) Purity and source not given.	
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliguots of saturatured solu-		
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).	

COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) 1-Propanol; C ₃ H ₈ O; [71-23-8] VARIABLES: T/K = 298	ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. J. Chem. Eng. Data <u>1993</u> , 38, 389-392. PREPARED BY: W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	<i>*</i> 1	
25.0 0.9994	0.000591	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).	
COMPONENTS	OPTOTNAL MEASUREMENTS :	
---	--	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 2-Propanol; C₃H₈O; [67-63-0]</pre>	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A. Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.9996	0.000411	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Anderson, B.D.	
(2) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C c ₁ /	(mol dm ⁻³)	
25.0 0.0	0950	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) puriss, 99.5 %, Fluka Chemical Corpora- tion, Ronkonkoma, New York, USA, was stored over molecular sieves to remove trace water.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (relative error; compiler).	

COMPONENTS: ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; (1) Anthracene; C14H10; [120-12-7] Trejo, J.; Acree, W.E., Jr. (2) 1-Butanol; C₄H₁₀O; [71-36-3] J. Chem. Eng. Data 1993, 38, 389-392. VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C x₁ x₂ 0.9992 0.000801 25.0 AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by (2) HPLC Grade, 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 356 nm.

ESTIMATED ERRORS:

 $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.	
(2) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6]	J. Chem. Eng. Data <u>1994</u> , 39, 114-116.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	<i>x</i> 1	
25.0 0.9994	0.000585	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).	

CONDONENT C :	OPTOTNAL MEASUREMENTS:
COMPONENTS:	URIGINAL MERSORIFIEMIS.
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2) 2-Methyl-1-propanol; C ₄ H ₁₀ O; [78-83-1]	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x ₁
25.0 0.9995	0.000470
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1.3$ % (relative error).

COMONEDING		
	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.	
(2) 3-Methyl-1-butanol; C ₅ H ₁₂ O; [123-51-3]	J. Chem. Eng. Data, in press.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.9993	0.000727	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1.3 $ (relative error).	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Anderson, B.D. Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_{1}/(mol dm^{-3})$		
25.0 0.0	0.0140	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flags, weighed and diluted with methanol	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). c ₁ : \pm 3 % (relative error; compiler).	

COMPONENTS:	OPTOTNAL MEASUREMENTS .	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. <u>1985</u> , 19, 522-529.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /(mol dm ⁻³)	
25.0 0.01	0.0118	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection. Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphage column	 Highest available commercial purity, specific chemical supplier not given, was used as received. 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received. 	
	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). c ₁ : \pm 3 % (relative error; compiler).	

CONDONENTS	ORIGINAL MEASUREMENTS:	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. Environ. Sci. Technol. <u>1990</u> , 24, 639-646.	
VARIABLES:	PREPARED BY:	
T/K = 296	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_1/(mol dm^{-3})$		
23.0 0.0	0.0117	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	 Purity not given, commercial sample of unspecified source, was used as received. 	
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.	
fluorescence or uv detection.	ESTIMATED ERRORS:	
	$T/K: \pm 1.$ $c_1: \pm 5$ % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A. <i>Fluid Phase Equilibr</i> . <u>1994</u> , <i>92</i> , 233-253.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	* 1	
25.0 0.9978	0.002160	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. 	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1: \pm 1 $ (relative error).	

COMPONENTS:

(1) Anthracene; C₁₄H₁₀; [120-12-7]
 (2) 1-Octanol; C₈H₁₈O; [111-87-5]

EVALUATOR:

W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) June, 1994

CRITICAL EVALUATION:

Anthracene solubilities in 1-octanol were retrieved from papers by Pinal *et al.* (1), Miller *et al.* (2), Acree *et al.* (3), and Anderson (4). All four studies report the solubility at only a single temperature, either 296 K (1) or 298 K (2-4). In the case of both Miller *et al.* and Anderson, the published molarity solubilities were converted to mole fraction values of $x_1 = 0.00222$ and $x_1 = 0.00187$ using molar volumes of $V_1 =$ 150 cm³ mol⁻¹ and $V_2 = 158.30$ cm³ mol⁻¹ for anthracene and 1-octanol, respectively. The arithmetic average of the three reported solubilities at 298.15 K, $x_1 = 0.00208$ ± 0.00019 is the recommended value for the mole fraction solubility of anthracene in 1-octanol.

REFERENCES

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    Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. Environ. Sci.
Technol. 1990, 24, 639.
    Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay D. Environ. Sci.
Technol. 1985, 19, 522.
    Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A. Fluid Phase Equilibr. 1994, 92,
233.
    Anderson, B.D., Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, 1978.
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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Smutek, M.; Fris, M.; Fohl, J.
(2) Phenol; C ₆ H ₆ O; [108-95-2]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 313	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x 1
40.0 0.9951	0.00487
AUXILIA	RY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in close glass container and allowed to equilibrat for several hours at constant temperature Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. (2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:
	T/K: precision \pm 0.05. x ₁ : \pm 3 % (relative error; compiler).

COMPONENTS	ORIGINAL MEASUREMENTS:	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) 1-Hydroxy-2-methylbenzene; C₇H₈O; [95-48-7]</pre>	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. Environ. Sci. Technol. <u>1990</u> , 24, 639-646.	
VARIABLES:	PREPARED BY:	
<i>T/K</i> = 296	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_{1}/(mol dm^{-3})$		
23.0 0.0	23.0 0.0308	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.	
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.	
fluorescence or uv detection.	ESTIMATED ERRORS:	
	T/K: \pm 1. c ₁ : \pm 5% (relative error; compiler).	

COMPONENTS	ORTGINAL WEASUREWENTS .
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Smutek, M.; Fris, M.; Fohl, J.
(2) 2-Propanone; C ₃ H ₆ O; [67-64-1]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	×1
20.0 0.9969	0.00313
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

VARIABLES:

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COMPONENTS:

T/K = 298

EXPERIMENTAL VALUES

(1) Anthracene; C14H10; [120-12-7]

(2) 2-Propanone; C₃H₈O; [67-64-1]

t/°C	<i>x</i> 2 ^a	<i>*</i> 1 ^a
25.0	0.9957	0.00432

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

AUXILIARY INFORMATION

ORIGINAL MEASUREMENTS:

Bull. Soc. Chim. Belgique <u>1936</u>, 45, 667-677.

Mahieu, J.

PREPARED BY:

W.E. Acree, Jr.

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance.	(1) Purity and source not given.	
	(2) Purity and source not given.	
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliquots of saturatured solu-		
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.5 (compiler). x_1 : \pm 5 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-17-7] (2) 2-Propanone; C₃H₆O; [67-64-1]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.954 0.04	46
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

CONDONENTS	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-17-7] (2) 2-Butanone; C ₄ H ₈ O; [78-93-3]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0,9953 0,0	047
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. x_1 : \pm 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Acetonitrile; C₂H₃N; [75-05-8]</pre>	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.		
VARIABLES:	PREPARED BY:		
<i>T</i> /K = 296	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C	mol dm ⁻³)		
23.0 0.00	973		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	 Purity not given, commercial sample of unspecified source, was used as received. 		
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.		
fluorescence or uv detection.	ESTIMATED ERRORS:		
	$T/K: \pm 1$. $c_1: \pm 5$ % (relative error; compiler).		

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C₁₄H₁₀; [120-12-7] Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun., <u>1967</u>, 32, 931-943. (2) Carbon disulfide; CS₂; [75-15-0] PREPARED BY: VARIABLES: T/K = 293W.E. Acree, Jr. EXPERIMENTAL VALUES t/⁰C **x**1 x2 20.0 0.9913 0.00872 . AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE

METHOD: APPARATUS/PROCEDURE	SOURCE AND PORITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance.	(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane
Excess solute and solvent placed in closed class container and allowed to equilibrate	to give a final purity of 98.3 %.
for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	(2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:
	T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

[<u></u>						
COMPONENTS :			ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]			Doane, E.P.; Drickamer, H.G.			
(2) Carbon disulfide; CS ₂ ; [75-15-0]			J. Phys. Cl	1955, 1955, 1	59, 454-457.	
VARIABLES:			PREPARED BY:	1		
T/K ≠ 298, Pressure			W.E. Acree,	Jr.		
EXPER	IMENTAL VAL	UES				
	P/atm	x2	<i>x</i> 1	P/atm	*2	<i>x</i> 1
	1	0.9916	0.0084	2000	0.9973	0.0027
	240	0.9930	0.0070	4000	0.9987	0.0013
	500	0.9941	0.0059			
	1000	0.9959	0.0041			
AUXILIARY		INFORMATION				
METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF MA	TERIALS:		
Constant temperature bath, analytical balance and high pressure equipment.		(1) Purest Company used as	grade, East Y, Rochester s received.	man Kodak Chemical , New York, USA, was		
Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount of saturated solution removed, solvent evaporated to dryness, and con- tration determined from weight of solid residue.		(2) C.P. g phospho	rade, J.T. B prous pentox	aker, was dried over ide and distilled.		
		ESTIMATED E T/K: precis $x_1: \pm 1-3$ % ± 10 %	RRORS: sion <u>+</u> 0.1. s at atmospherat the high	eric pressure, and er pressures.		

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Anthracene; C₁₄H₁₀; [120-17-7] (2) Acetic anhydride; C₄H₆O₃; [108-24-7] 	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.9972 0.0	028
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

ORIGINAL MEASUREMENTS:	
Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
PREPARED BY:	
W.E. Acree, Jr.	
001	
021	
INFORMATION	
SOURCE AND PURITY OF MATERIALS:	
 Purity and chemical source not speci- fied in paper. 	
(2) Purity and chemical source not speci- fied in paper.	
ESTIMATED ERRORS:	
T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Dimethyl sulfoxide; C₂H₆SO; [67-68-5]</pre>	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. Environ. Sci. Technol. <u>1990</u> , 24, 639-646.			
VARIABLES:	PREPARED BY:			
T/K = 296	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C c ₁ /	(mol dm ⁻³)			
23.0 0.0	315			
AUXILIARY	AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	 Purity not given, commercial sample of unspecified source, was used as received. 			
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.			
fluorescence or uv detection.	ESTIMATED ERRORS:			
	$T/K: \pm 1.$ $c_1: \pm 5$ % (relative error; compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.			
(2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂ ª	×1 ^a			
25.0 0.9897	0.01032			
^a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.				
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer, and a precision balance.	(1) Purity and source not given.			
Excess solute and solvent placed in closed glass containers and allowed to equili-	(2) Purity and Bource not given.			
brate for several hours at constant temperature. Aliquots of saturatured solu-				
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained	ESTIMATED ERRORS:			
after solvent had evaporated.	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.		
(2) Mitrodenzene; $C_6H_5NO_2$; [98-95-3]	Environ. Sci. Technol. <u>1990</u> , 24, 639–646.		
VARIABLES:	PREPARED BY:		
T/K = 296	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C c ₁ /(mol dm ⁻³)		
23.0 0.0	0.0738		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear super- natant solution was analyzed by reversed- phase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.		
fluorescence or uv detection.	ESTIMATED ERRORS:		
	$T/K: \pm 1.$ $c_1: \pm 5$ % (relative error; compiler).		

-			1		
COMPONENTS:			ORIGINAL N	EASUREMENTS:	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Nitrobenzene; C₆H₅NO₂; [98-95-3]</pre>		Srivastava, R.D.; Gupta, P.D. <i>J. Indian Chem. Soc</i> . <u>1967</u> , 44, 960-963.			
					VARIABLES:
Temperature			W.E. Acre	ee, Jr.	
EXPERIMENTAL V	/ALUES				
T/K	*2	x 1	T/K	×2	x 1
286.2	0.9931	0.00688	307.4	0.9846	0.01545
289.8	0.9908	0.00916	308.2	0.9839	0.01614
296.2	0.9890	0.01104	313.0	0.9811	0.01892
298.2	0.9885	0.01152	_		
		AUXILIARY	INFORMATION	1	
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE ANI	D PURITY OF M	ATERIALS:
Constant temp thermometer.	perature bath	and a precision	(l) Purit Unite subli	y not given, d Kingdom, w .med.	British Drug Houses, as recrystallized and
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(2) Purit was c	y not given, dried and dis	British Drug Houses, tilled.	
		ESTIMATED	ERRORS:		
		T/K: pred	ision <u>+</u> 0.1.		
		x ₁ : ± 3 %	(relative e	rror, Compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mahieu, J.		
(2) Aniline; C ₆ H ₇ N; [62-53-3]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.		
VARIABLES:	PREPARED BY:		
T/K = 298 and 313	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂ ^a	×1 ^a		
25.0 0.9961	0.00390		
40.0 0.9923	0.00773		
^a computed by compiler from published so solubilities, which were expressed as we solute per 100 grams of solvent.	lvent compositions and solute eight percent and grams of		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer,	(1) Purity and source not given.		
and a precision balance.	(2) Purity and source not given.		
Excess solute and solvent placed in closed glass containers and allowed to equili- brate for several hours at constant temperature. Aliguots of saturatured solu-			
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.	ESTIMATED ERRORS:		
	T/K: precision \pm 0.5 (compiler). x ₁ : \pm 5 % (relative error; compiler).		

COMPONENTS:			ORIGINAL M	EASUREMENTS:	
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Pyridine; C₅H₅N; [110-86-1] VARIABLES:</pre>		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534. PREPARED BY:			
					Temperature
EXPERIMENTAL V	ALUES				
T/K	×2	×1	T/K	x2	x 1
313.5	0.9833	0.0167	353.1	0.9470	0.0530
326.7	0.9758	0.0242	359.0	0.9415	0.0585
337.4	0.9674	0.0326			
344.5	0.9603	0.0397			
		AUXILIARY	INFORMATION	8	
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(1) 99.99 Milwi talli (2) Gold Compa	9+ %, Aldrich aukee, Wiscor ized from tol Label, 99.9+ any, was used	 Chemical Company, nsin, USA, was recrys- uene. %, Aldrich Chemical l as received. 	
		$\begin{bmatrix} T/K: & pre \\ x_1: \pm 0.0 \end{bmatrix}$	ERRORS: cision <u>+</u> 0.1. 0003.		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Pyridine; C ₅ H ₅ N; [110-86-1]	Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.		
VARIABLES:	PREPARED BY:		
T/K = 293 and 333	W.E. Acree, Jr.		
EIPERIMENTAL VALUES	,		
t/°C x ₂	<i>x</i> ₁		
20.0 0.9917	0.00834		
60.0 0.9716	0.0284		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %. 99 %, Commercial sample, source and purification method was not specified. 		
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).		

COMPONENT S:	ORIGINAL MEASUREMENTS :
(1) Anthracene; C ₁₄ H ₁₀ ; [120-17-7] (2) Pyridine; C ₅ H ₅ N; [110-86-1] VARIABLES:	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation) PREPARED BY:
1/K - See Delow	, w.2. Acree, 51.
EXPERIMENTAL VALUES x ₂ x ₁ 0.989 0.03	11
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-17-7] (2) Quinoline; C₉H₇N; [91-22-5]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	•
x ₂ x ₁	
0.989 0.0	11
AUXILIARY	INFORMATION .
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	$x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Thiophene; C₄H₄S; [110-02-1] </pre>	Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.
VARIADLED:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
T/K x ₂ x ₁	T/K x ₂ x ₁
297.4 0.9895 0.0105	351.8 0.9506 0.0494
317.9 0.9798 0.0202	358.1 0.9430 0.0570
332.9 0.9697 0.0303	
337.0 0.9659 0.0341	
AUX	ILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a preci thermometer. Mixtures of known concentrations seal in glass ampoules and placed in const temperature to equilibrate. Samples were rotated while bath temperature s increased. Solubility determined by	sion (1) 99.99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrys- tallized from toluene. (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.
noting the temperature at which the 1 trace of solid solute disappeared.	ast ESTIMATED ERRORS:
	$T/K:$ precision \pm 0.1. $x_1: \pm 0.0003.$

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-17-7] (2) Methoxybenzene; C₇H₈O; [100-66-3]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.9898 0.0	102
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS: T/K: Unknown.
	$x_1: \pm v \in (relative error; compiler).$

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-17-7] (2) 1-Methyl-2-pyrrolidinone; C₅H₉NO; [872-50-4]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
	25
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Anthracene; C₁₄H₁₀; [120-17-7] N,N-Dimethylacetamide; C₄H₉NO; [127-19-5] 	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	<u>.</u>
x ₂ x	1
0.986 0	.014
AUXILIA	RY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS :	ORIGINAL MEASUREMENTS:
 (1) Anthracene; C₁₄H₁₀; [120-17-7] (2) N,N-Dimethylformamide; C₃H₇NO; [68-12-2] 	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
x ₂ x ₁	
0.991 0.00)9
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

CONTONETTE .	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-17-7] (2) Tetramethylene sulfone; C₄H₈O₂S; [126-33-0] VARIABLES:</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation) PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES x ₂ x ₁ 0.9964 0.0 ⁷	036
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	URIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
<pre>(2) Tributyl phosphate; C₁₂H₂₇O₄P; [126-73-8]</pre>	Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
x ₂ x ₁	
	11
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Shinomiya, C.
<pre>(2) 1,2,3,5-Tetranitrobenzene; C₆H₂N₄O₈; [3698-53-1]</pre>		J. Chem. Soc. Japan <u>1940</u> , 15, 259-270.
VAR IABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
T/K	<i>x</i> ₂	x1
399.2	1.000	0.000
398.2	0.935	0.065
418.2	0.842	0.158
436.2	0.693	0.307
442.2	0.604	0.396
444.2	0.487	0.513
441.7	0.430	0.570
449.2	0.354	0.646
459.2	0.301	0.699
462.2	0.271	0.729
490.2	0.000	1.000
AUXILIARY INFORMATION		INFORMATION
No experimental details g	iven in paper.	 (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not
		specified in paper.
		ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). $x_1: \pm 0.002$ (Compiler).

CONDONENTS	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Singh, N.P.; Shukla, B.M.	
(2) 2,4,6-Trinitrophenol; C ₆ H ₃ N ₃ O ₇ ; [88-89-1]	Cryst. Res. Technol. <u>1985</u> , 20, 345-349.	
VARIABLES:	PREPARED BY:	
	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
Phase equilibrium data not given in cit	ed paper. Authors report formation of a	
1:1 anthracene - 2,4,6-trinitrophenol m	olecular compound having a melting point	
temperature of 413.2 K. Two eutectic p	oints occur at $x_1 = 0.1017$ and $T/K = 382.7$,	
and at $x_1 = 0.6250$ and $T/K = 403.2$.		
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Binary mixtures were prepared by weight. Melting and thaw point temperatures	(1) Purity and chemical source not speci- fied in paper.	
al. (see J. Cryst. Growth <u>1977</u> , 40, 329).	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.0002 (Compiler).	

Components :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Acree, W.E., Jr.
(2) t-Butylcyclohe [3178-22-1]	exane; C ₁₀ H ₂₀ ;	J. Chem. Eng. Data <u>1994</u> , 39, 117-118.
(3) 2,2,4-Trimethy [540-84-1]	lpentane; C ₈ H ₁₈ ;	
VARIABLES:		PREPARED BY:
T/K = 298, Solvent	composition	W.E. Acree, Jr.
EXPERIMENTAL VALUE: t = 25.0 °C	Sa	
x ₇ ^(s)	x,	x,
0.0000	0.0000	0.001978
0.1093	0.1091	0.001899
0.2115	0.2111	0.001809
0.3862	0.3856	0.001651
0.5049	0.5041	0.001536
0.6142	0.6133	0.001429
0.8099	0.8089	0.001249
0.8961	0.8951	0.001163
1.0000	0.9989	0.001074
<u>1</u>	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mi weight. Excess so in amber glass bo equilibrate for a temperature. Att was verified by a measurements and brium from super saturated solution a coarse filter flasks, weighed Concentrations do metrically at 350	Lixtures were prepared by plute and solvent placed ottles and allowed to several days at constant tainment of equilibrium several repetitive by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. etermined spectrophoto- 6 nm.	 (2) 99 %, Aldrich Chemical Company. (3) HPLC Grade, 99.7 %, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_3^{(S)}: \pm 0.0001.$ $x_1: \pm 1 $ (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) n -torange C H (110-54-3)	Trejo, J.; Acree, W.E., Jr.
(3) 1-Propanol; C ₃ H ₈ O; [71-23-8]	J. Chem. Eng. Data <u>1993</u> , 38, 389-392.
/ARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	
x ₃ ^(s) x ₃	x ₁
0.0000 0.0000	0.001274
0.1751 0.1749	0.001288
0.3162 0.3158	0.001237
0.5447 0.5441	0.001071
0.6331 0.6325	0.000990
0.7297 0.7290	0.000898
0.8712 0.8706	0.000740
0.9411 0.9435	0.000661
1.0000 0.9994	0.000591
AUXILIA	
GETHOD: 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	 SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ mole %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical
equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
flasks, weighed and diluted with methano. Concentrations determined spectrophoto- metrically at 356 nm.	

COMPONENTS:			ORIGINAL MEASUREMENTS:
 Anthracene; C₁₄H₁₀; [120-12-7] n-Heptane; C₇H₁₆; [142-82-5] 1-Propanol; C₃H₈O; [71-23-8] 		[120-12-7] [142-82-5] [71-23-8]	Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. <i>J. Chem. Eng. Data</i> <u>1993</u> , <i>38</i> , 389-392.
VARIA	BLES:		PREPARED BY:
T/K	= 298, Solvent con	nposition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C			
	x ₁ ^(s)	Xz	X1
i	0.0000	0.0000	0.001571
	0.1719	0.1716	0.001566
	0.3272	0.3267	0.001456
	0.5674	0.5667	0.001182
	0.6622	0.6615	0.001077
	0.7444	0.7437	0.000953
	0.8824	0.8817	0.000762
	0.9398	0.9392	0.000681
ļ	1.0000	0.9994	0.000591
	the ternary solut	ion.	
		AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		EDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		bath, calorimetric ltraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		es were prepared by and solvent placed s and allowed to al days at constant ent of equilibrium al repetitive pproaching equili- ation. Aliquots of ransferred through tared volumetric iluted with methanol. ined spectrophoto-	 (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: $T/K: \pm 0.05.$ $x_3^{(5)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

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COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) n-Octane; C ₈ H ₁₈ ; [111-65-9] (3) 1-Propanol; C ₃ H ₈ O; [71-23-8]	ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. J. Chem. Eng. Data <u>1993</u> , 38, 389-392.	
VARIABLES: T/K = 298, Solvent composition	PREPARED BY: W.E. Acree, Jr.	
EXPERIMENTAL VALUES ^a t = 25.0 °C		
$x_3^{(s)}$ x_3 0.0000 0.0000 0.1908 0.1905 0.3483 0.3477 0.5892 0.5884 0.6806 0.6798 0.7661 0.7653 0.8939 0.8932 0.9477 0.9471 1.0000 0.9994 $a_{x_3}^{(s)}$: initial mole fraction of binary fraction solubility of the solute; x_3 : monthe ternary solution.	<pre>41 0.001838 0.001779 0.001632 0.001300 0.001145 0.001013 0.000784 0.000682 0.000591 solvent mixture; x1: mole mole fraction of component 3 in</pre>	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	 (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 Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS: T/K: ± 0.05. x₃⁽⁵⁾: ± 0.0001. 	
	$x_1: \pm 1$ % (relative error).	

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COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; (C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Teng, IL.; Martinez, E.;
(2) Cyclohexane;	C ₆ H ₁₂ ; [110-82-7]	Trejo, J.; Acree, W.E., JL.
(3) 1-Propanol; (C ₃ H ₈ O; [71-23-8]	J. Chem. Eng. Dala <u>2222</u> , 30, 303 392.
VARIABLES:		PREPARED BY:
<i>T</i> /K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU t = 25.0 °C	ES ^a	
x _z ^(s)	Xz	x,
0.0000	0.0000	
0.1335	0.1333	0.001576
0.2567	0.2563	0.001543
0.4886	0.4880	0.001288
0.5890	0.5883	0.001150
0.6893	0.6886	0.001010
0.8511	0.8504	0.000795
0.9226	0.9220	0.000699
1.0000	0.9994	0.000591
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ature bath, calorimetric an ultraviolet/visible er.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess s in amber glass b	aixtures were prepared by solute and solvent placed sottles and allowed to	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
equilibrate for temperature. At was verified by	several days at constant tainment of equilibrium several repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05. x_3^{(s)}: \pm 0.0001. x_1: \pm 1 % (relative error).$

		t
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Teng, IL.; Martinez, E.;
(2) Methylcycloh (108-87-2)	exane; C ₇ H ₁₄ ;	J. Chem. Eng. Data 1993, 38, 389-392.
<pre>(3) 1-Propanol;</pre>	C _z H _e O; {71-23-8]	<u> </u>
VARIABLES:		PREPARED BY:
T/K = 298, Solve	ent composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	res ^a	
x_(s)	X7	X1
0.0000	0.0000	0.001649
0.1539	0.1536	0.001697
0,2943	0.2938	0.001578
0.5326	0.5319	0.001294
0.6305	0.6298	0-001154
0.7206	0.7199	0.001018
0.8687	0.8680	0.000781
0 9329	0.9322	0,000687
1 0000	0.9994	0,000591
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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		<pre>(2) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
		(3) 99+ %, anhydrous, Aldrich Chemical Company.
was verified by measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35	several repetitive d by approaching equili- ssaturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. determined spectrophoto- 66 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

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COMPONENTS:			ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		; [120-12-7]	Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Treio, J.; Acree, W.E., Jr.
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ;		ntane; C ₈ H ₁₈ ;	J. Chem. Eng. Data 1993, 38, 389-392.
(3)	1-Propanol; C ₃ H ₂ O	; [71-23-8]	
VARI	TABLES:		PREPARED BY:
T/K	K = 298, Solvent co	mposition	W.E. Acree, Jr.
EIPE t =	RIMENTAL VALUES ^a • 25.0 °C		
	x3 ^(s)	*3	×1 .
	0.0000	0.000	0.001074
	0.2141	0.2139	0.001089
	0.3510	0.3506	0.001057
	0.5891	0.5886	0.000929
	0.6884	0.6878	0.000862
	0.7911	0.7905	0.000783
	0.8968	0.8962	0.000693
	0.9454	0.9448	0.000649
	1.0000	0.9994	0.000591
		AUXILIARY	INFORMATION
METEOD: APPARATUS/PROCEDURE		CEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		bath, calorimetric ultraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bi	Binary solvent mixtures were prepared by weight. Excess solute and solvent placed		(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		ral days at constant ment of equilibrium ral repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
		approaching equili- ration. Aliquots of transferred through tared volumetric diluted with methanol. mined spectrophoto-	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
			ESTIMATED ERRORS:
			$T/K: \pm 0.05. x_3^{(s)}: \pm 0.0001. x_1: \pm 1 % (relative error).$

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COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1] (3) l=Propagal; C H 0; [71-23-8]	ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Acree, W.E., Jr. J. Chem. Eng. Data <u>1994</u> , 39, 117-118.
VARIABLES: T/K = 298, Solvent composition	PREPARED BY: W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	
$x_3^{(s)}$ x_3 0.0000 0.0000 0.2089 0.2085 0.3695 0.3688 0.6061 0.6052 0.7002 0.6993 0.7780 0.7771 0.9021 0.9014 0.9537 0.9530 1.0000 0.9994 * $x_3^{(s)}$: initial mole fraction of binary fraction solubility of the solute; x_3 : m the ternary solution.	<pre>x1 0.001978 0.001958 0.001792 0.001423 0.001250 0.001100 0.000824 0.000706 0.000591 solvent mixture; x1: mole mole fraction of component 3 in</pre>
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically 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.
	$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
(2) n-Hexane; C	6 ^H 14; [110-54-3]	Fluid Phase Equilibr. 1994. 92. 233-253
(3) 2-Propanol;	С ₃ H ₈ O; [67-63-0]	11010 Fildse Equilibri (<u>1994</u>) 727 255-255.
VARIABLES:		PREPARED BY:
<i>T/K = 298, Solv</i>	vent composition	W.E. Acree, Jr.
EXPERIMENTAL VAL $t = 25.0$ °C	JUES ^a	
x3 ^(s)	×3	x ₁
0.0000	0.0000	0.001274
0.1739	0.1737	0.001271
0.3076	0.3072	0.001201
0.5342	0.5337	0.000987
0.6314	0.6308	0.000873
0.7185	0.7179	0.000767
0.8700	0.8695	0.000581
0.9391	0.9386	0.000490
1.0000	0.9996	0.000411
	AUXILIARY	INFORMATION
METHOD: APPARAT	US/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempe thermometer, a spectrophotome	rature bath, calorimetric nd an ultraviolet/visible ter.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent	mixtures were prepared by solute and solvent placed	(2) 99+ mole %, Aldrich Chemical Company.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		(3) 99+ %, anhydrous, Aldrich Chemical Company.
		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K_{i} \pm 0.05. \\ x_{3}^{(s)}: \pm 0.0001. \\ x_{1}: \pm 1.5 \ (relative error).$

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COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) n-Heptane; C ₇ H ₁₆ ; [142-82-5] (3) 2-Propanol; C ₃ H ₈ O; [67-63-0]		ORIGINAL MEASUREMENTS: Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.
		Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
VARIABLES:		PREPARED BY:
T/K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU t = 25.0 °C	ES ^a	
x3 ⁽³⁾	x 3	<i>x</i> 1
0.0000	0.0000	0.001571
0.1851	0.1848	0.001499
0.3256	0.3252	0.001371
0.5575	0.5569	0.001102
0.6607	0.6601	0.000956
0.7381	0.7375	0.000836
0.8861	0.8856	0.000603
0.9416	0.9411	0.000509
1.0000	0.9996	0.000411
	AUXILIARY	INFORMATION
METHOD: APPARATUS	/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ture bath, calorimetric an ultraviolet/visible gr.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess s in amber glass b	ixtures were prepared by olute and solvent placed ottles and allowed to	(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive		(3) 99+ %, anhydrous, Aldrich Chemical Company.
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.	
		ESTIMATED ERRORS:
		$T/K: \pm 0.05. \\ x_3^{(s)}: \pm 0.0001. \\ x_1: \pm 1.5 \ \text{(relative error)}.$

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COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
(2) n-Octane; C ₈ 1	H ₁₈ ; [111-65-9]	S.A.
(3) 2-Propanol;	С ₃ H ₈ O; [67-63-0]	Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
VARIABLES:		PREPARED BY:
<i>T/</i> K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	ES ^a	
2 - 25.0 -C	¥-	x.
<u>s</u> 0, 0000		0.001838
0.2157	0.2153	0.001690
0.3580	0.3574	0.001540
0,5840	0.5833	0.001206
0.6874	0.6867	0.001025
0,7670	0.7663	0.000868
0.8928	0.8922	0.000622
0.9478	0.9473	0.000515
1 0000	0 9996	0 000411
	AUXILIARY	INFORMATION
METHOD: APPARATUS	S/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	uture bath, calorimetric 1 an ultraviolet/visible 27.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		(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:
		$\begin{array}{l} T/K: \pm 0.05. \\ x_3^{(s)}: \pm 0.0001. \\ x_1: \pm 1.5 \ (relative \ error). \end{array}$

CONTROLIENTIS		
COMPONENTS:		Deres W.R. In . Sweigene D.T Sweigen
(1) Anthracene; ($C_{14}H_{10}; [120-12-7]$	Acree, W.E., Jr.; Zvalgzne, A.I.; Tucker, S.A.
(2) Cyclonexane;	$C_{6}H_{12};$ [110-82-7]	Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
(3) 2-Propanol; (C ^{3H8} O; [61-63-0]	
VARIABLES:		PREPARED BY:
T/K = 298, Solve:	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	ES ^a	
x ₁ ^(s)	<i>x</i> ₁	x,
0.0000	0.0000	0.001553
0.1430	0.1428	0.001568
0.2666	0.2662	0.001474
0.4882	0.4876	0.001213
0.5897	0.5891	0.001051
0.6817	0.6811	0.000899
0.8463	0.8458	0.000639
0.9239	0.9234	0.000519
1,0000	0,9996	0.000411
	AUXILIARY	INFORMATION
METHOD: APPARATUS	/ PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ture bath, calorimetric an ultraviolet/visible r.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m.	ixtures were prepared by	(2) HPLC Grade, 99.9+ %, Aldrich Chemical
in amber glass b equilibrate for	ottles and allowed to several days at constant	(3) 99+ %, anhydrous, Aldrich Chemical
temperature. At	tainment of equilibrium	Company.
measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35	by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. etermined spectrophoto- 6 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K; \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5$ % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
(2) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2]	Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
(3) 2-Propanol; C ₃ H ₈ O; [67-63-0]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a $t = 25.0 ^{\circ}C$	
x ₁ (s) x ₁	x,
0.0000 0.0000	0.001649
0.1518 0.1515	0.001683
0.2965 0.2960	0.001536
0.5234 0.5228	0.001226
0.6234 0.6227	0.001055
0.7170 0.7164	0.000887
0.8649 0.8644	0.000631
0.9375 0.9370	0.000508
1.0000 0.9996	0.000411
AUXILIA	RY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through	 (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.
a coarse filter into tared volumetric flasks, weighed and diluted with methanol Concentrations determined spectrophoto- metrically at 356 nm.	1.
	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5 % (relative error).$

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ;	S.A.
(3) 2-Propanol: C_H_O: $(67-63-0)$	riulu rilase Equilibri : 1224, 32, 255-255.
(0, 1, 1, 0, 2, 0, 3, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a	
x_(s) x_	х.
0.0000 0.0000	0.001074
0.1997 0.1995	0.001054
0.3535 0.3532	0.000988
0.5865 0.5860	0.000839
0.6809 0.6804	0.000751
0.7676 0.7671	0.000664
0.8932 0.8927	0.000535
0.9492 0.9488	0.000471
1.0000 0.9996	0.000411
AUXILIARY	INFORMATION
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed	(2) HPLC Grade, 99.7 %, Aldrich Chemical
in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium	<pre>(3) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS:
	$T/X: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5$ % (relative error).

Components:			ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1]		e; C ₁₀ H ₂₀ ;	J. Chem. Eng. Data <u>1994</u> , 39, 117-118.
(3)	2-Propanol; C ₃ H ₈ O;	[67-63-0]	
VARI	ABLES:		PREPARED BY:
T/K	= 298, Solvent co	mposition	W.E. Acree, Jr.
EXPE t =	RIMENTAL VALUES ^a 25.0 °C		
	x ₃ ^(s)	<i>x</i> ₃	x ₁
	0.0000	0.0000	0.001978
	0.2154	0.2150	0.001978
	0.3666	0.3660	0.001760
	0.5948	0.5940	0.001335
	0.6912	0.6904	0.001152
	0.7744	0.7737	0.000948
	0.8963	0.8957	0.000660
	0.9537	0.9532	0.000526
	1.0000	0.9996	0.000411
		AUXILIARY	INFORMATION
METH	OD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		bath, calorimetric ltraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		es were prepared by and solvent placed s and allowed to al days at constant	 (2) 99 %, Aldrich Chemical Company. (3) 99+ %, aphydrous, Aldrich Chemical
		nent of equilibrium al repetitive	Company.
		pproaching equili- ation. Aliquots of ransferred through tared volumetric liluted with methanol. lined spectrophoto-	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
			ESTIMATED ERRORS:
			$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).
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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.		
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	J. Chem. Eng. Data <u>1993</u> , 38, 389-392.		
(3) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]			
VARIABLES:	PREPARED BY:		
T/K = 298, Solvent composition	W.E. Acree, Jr.		
EXPERIMENTAL VALUES ^a t = 25.0 °C			
x ₃ ^(s) x ₃	x 1		
0.0000 0.0000	0.001274		
0.1460 0.1458	0.001316		
0.2668 0.2665	0.001310		
0.4876 0.4870	0.001218		
0.5800 0.5793	0.001162		
0.6804 0.6797	0.001068		
0.8479 0.8471	0.000931		
0.9247 0.9239	0.000857		
1.0000 0.9992	0.000801		
i l AUX	ILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetr: thermometer, and an ultraviolet/visible spectrophotometer. Binary solvent mixtures were prepared weight. Excess solute and solvent place in amber glass bottles and allowed to equilibrate for several days at consta temperature. Attainment of equilibriu was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred throug a coarse filter into tared volumetric flasks, weighed and diluted with metha Concentrations determined spectrophoto metrically at 356 nm.	<pre>ic (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ mole %, Aldrich Chemical Company. (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS: T/K; ± 0.05. x₃^(S): ± 0.0001. x₁: ± 1 % (relative error).</pre>		

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.: Acree, W.E., Jr.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]		J. Chem. Eng. Data 1993, 38, 389-392.
(3) 1-Butanol; C ₄ H ₁₀	₀ 0; [71-36-3]	
VARIABLES:		PREPARED BY:
T/K = 298, Solvent	composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	1	
x3 ^(s)	<i>x</i> 3	x1
0.0000	0.000	0.001571
0.1562	0.1560	0.001576
0.2876	0.2872	0.001511
0.5171	0.5164	0.001333
0.6174	0.6166	0.001230
0.7033	0.7025	0.001142
0.8622	0.8614	0.000972
0.9315	0.9307	0.000886
1.0000	0.9992	0.000801
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PH	ROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature thermometer, and an spectrophotometer.	re bath, calorimetric n ultraviolet/visible	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixt	tures were prepared by te and solvent placed	(2) HPLC Grade, 99.7+ %, Aldrich Chemical
in amber glass both equilibrate for sev temperature. Attai	tles and allowed to veral days at constant Inment of equilibrium	 (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) n-Octane; C ₈ H ₁₈ ; [111-65-9] (3) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]		ORIGINAL MEASUREMENTS:
		Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. J. Chem. Eng. Data <u>1993</u> , 38, 389-392.
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALU	ES ^a	<u> </u>
x, (s)	X7	x,
0.0000	0.0000	0.001838
0.1645	0.1642	0.001828
0.3070	0.3065	0.001725
0.5368	0.5360	0.001467
0.6389	0.6380	0.001336
0.7313	0.7304	0.001207
0.8738	0.8729	0.000998
0.9365	0.9357	0.000892
1.0000	0.9992	0,000901
a _{X3} (s): init fraction sol the ternary	ial mole fraction of binary ubility of the solute; x ₃ : m solution.	solvent mixture; x ₁ : mole nole fraction of component 3 in
^a x ₃ ^(s) : init fraction sol the ternary	ial mole fraction of binary ubility of the solute; x3: n solution.	solvent mixture; x ₁ : mole nole fraction of component 3 in
^a x ₃ ^(s) : init fraction sol the ternary	ial mole fraction of binary ubility of the solute; x3: m solution.	solvent mixture; x ₁ : mole mole fraction of component 3 in INFORMATION
<pre>* x₃(s): init fraction sol the ternary method: Apparatus</pre>	ial mole fraction of binary ubility of the solute; x3: m solution. AUXILIARY	SOURCE AND PURITY OF MATERIALS:
<pre>* x₃^(s): init fraction sol the ternary METHOD: APPARATUS Constant tempera thermometer, and spectrophotomete</pre>	AUXILIARY AUXILIARY B/PROCEDURE Autor bath, calorimetric an ultraviolet/visible J.	SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
<pre>* x₃^(s): init fraction sol the ternary METHOD: APPARATUS Constant tempera thermometer, and spectrophotomete Binary solvent m weight. Excess s in amber glass b equilibrate for</pre>	AUXILIARY AUXILIARY S/PROCEDURE AUXILIARY AUXILIARY AUXILIARY S/PROCEDURE AUXILIARY AUXILIA	<pre>solvent mixture; x₁: mole mole fraction of component 3 in INFORMATION SOURCE AND FURITY 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, 99.8t %, Aldrich Chemical</pre>
<pre>* x₃(s): init fraction sol the ternary METHOD: APPARATUS Constant tempera thermometer, and spectrophotomete Binary solvent m weight. Excess s in amber glass b equilibrate for temperature. At was verified by measurements and</pre>	AUXILIARY AUXILIARY B/PROCEDURE AUXILIARY B/PROCEDURE Aution calorimetric an ultraviolet/visible Br. Auxiliary A	<pre>solvent mixture; x_i: mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ %, anhydrous, Aldrich Chemical Company. (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company. (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company. Components 2 and 3 were stored over</pre>
<pre>* x₃^(s): init fraction sol the ternary METHOD: APPARATUS Constant tempera thermometer, and spectrophotomete Binary solvent m weight. Excess s in amber glass b equilibrate for temperature. At was verified by measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35</pre>	ial mole fraction of binary ubility of the solute; x ₃ : m solution. AUXILIARY S/PROCEDURE Ature bath, calorimetric an ultraviolet/visible r. dixtures were prepared by solute and solvent placed solute and solvent placed solutes and allowed to several days at constant trainment of equilibrium several repetitive by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. letermined spectrophoto- 6 nm.	<pre>solvent mixture; x₁: mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ %, anhydrous, Aldrich Chemical Company. (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company. (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use.</pre>
<pre>* x₃(s): init fraction sol the ternary METHOD: APPARATUS Constant tempera thermometer, and spectrophotomete Binary solvent m weight. Excess s in amber glass b equilibrate for temperature. At was verified by measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35</pre>	AUXILIARY AUXILIARY S/PROCEDURE ture bath, calorimetric an ultraviolet/visible er. dixtures were prepared by tolute and solvent placed ootles and allowed to several days at constant trainment of equilibrium several repetitive by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. etermined spectrophoto- 6 nm.	<pre>solvent mixture; x,: mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ %, anhydrous, Aldrich Chemical Company. (3) HPLC Grade, 99.8+ %, Aldrich Chemical Components 2 and 3 were stored over molecular sieves and distilled shortly before use.</pre>

02		
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Teng, IL.; Martinez, E.;
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		Trejo, J.; Acree, W.E., JL. T Chem Eng Data 1993. 38, 389-392.
(3) 1-Butanol; C	₄ H ₁₀ O; [71-36-3]	0. Crem. Day. Data <u>2000</u> , 00, 00, 001
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALU t = 25.0 °C	ES ^a	
x ₃ (s)	¥.	×,
0.0000	0.0000	0.001553
0.1151	0.1149	0.001622
0.2108	0.2105	0.001586
0.4380	0.4374	0.001414
0.5390	0.5383	0.001291
0.6811	0.6803	0.001152
0.8255	0.8247	0.000978
0.9086	0.9078	0.000895
1.0000	0.9992	0.000801
	AUXILIARY	INFORMATION
METHOD: APPARATUS	;/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ture bath, calorimetric an ultraviolet/visible sr.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess s in amber glass b	ixtures were prepared by solute and solvent placed sottles and allowed to	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
equilibrate for temperature. At was verified by	several days at constant tainment of equilibrium several repetitive	(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35	by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. letermined spectrophoto- 56 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(3)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

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Components :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Teng, IL.; Martinez, E.;
(2) Methylcyclohexane; C ₇ H ₁₄ ; (108-87-2)	J. Chem. Eng. Data 1993, 38, 389-392.
(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a	
x,(s) x ₁	X 4
0.0000 0.0000	0.001649
0.1358 0.1356	0.001710
0.2675 0.2671	0.001671
0.4783 0.4776	0.001453
0.5740 0.5732	0.001329
0.6764 0.6756	0.001193
0.8449 0.8441	0.000995
0.9221 0.9213	0.000892
1.0000 0.9992	0.000801
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed	(2) 99+ %, anhydrous, Aldrich Chemical
in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium	 (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_3^{(5)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]		J. Chem. Eng. Data <u>1993</u> , 38, 389-392.
(3) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]		
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C		
x ₃ (s)	<i>x</i> ₃	x,
0.0000	0.0000	0.001074
0.1567	0.1565	0.001125
0.3031	0.3028	0.001121
0.5376	0.5370	0.001051
0.6387	0.6381	0.000996
0.7330	0.7323	0.000956
0.8819	0.8811	0.000870
0.9443	0.9435	0.000838
1.0000	0.9992	0.000801
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PRO	OCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature thermometer, and an spectrophotometer.	a bath, calorimetric ultraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixto weight. Excess solut	res were prepared by e and solvent placed	(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

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COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.	
(2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1]	J. Chem. Eng. Data <u>1994</u> , 39, 117-118.	
(3) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]		
VARIABLES:	PREPARED BY:	
T/K = 298, Solvent composition	W.E. Acree, Jr.	
EXPERIMENTAL VALUES ^a t = 25.0 °C		
x ₃ ^(s) x ₃	×1	
0.0000 0.0000	0.001978	
0.1882 0.1878	0.001977	
0.3325 0.3319	0.001855	
0.5540 0.5531	0.001561	
0.6547 0.6538	0.001405	
0.7426 0.7417	0.001265	
0.8842 0.8833	0.001010	
0.9413 0.9404	0.000918	
1.0000 0.9992	0.000801	
AUXILIA	RY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURTTY OF WATERTALS.	
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol Concentrations determined spectrophoto- metrically at 356 nm.	 (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 Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS: T/K: ± 0.05. 	
	<pre>x3⁽⁵⁾: ± 0.0001. x1: ± 1 % (relative error).</pre>	

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COMPONENTS:		ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) n-Hexane; C₆H₁₄; [110-54-3] (3) 2-Butanol; C₄H₁₀O; [15892-23-6] VARIABLES: T/K = 298, Solvent composition</pre>		Zvaigzne, A.I.; Acree, W.E., Jr.
		J. Chem. Eng. Data <u>1994</u> , 39, 114-116.
		PREPARED BY:
		W.E. Acree, Jr.
EXPERIMENTAL VALU	ES ^a	
x3 ^(s)	<i>x</i> ₃	x,
0.0000	0.0000	0.001274
0.1432	0.1430	0.001311
0.2657	0.2654	0.001282
0.4851	0.4845	0.001169
0.5863	0.5857	0.001070
0.6820	0.6813	0.000969
0.8497	0.8490	0.000770
0.9249	0.9243	0.000676
1.0000	0.9994	0.000585
	AUXILIARY	INFORMATION
METHOD: APPARATUS	/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ture bath, calorimetric 1 an ultraviolet/visible r.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m	ixtures were prepared by	(2) 99+ mole %, Aldrich Chemical Company.
in amber glass b equilibrate for	solute and solvent placed sottles and allowed to several days at constant	(3) 99+ %, anhydrous, Aldrich Chemical Company.
temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5 $ % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	J. Chem. Eng. Data <u>1994</u> , 39, 114-116.
(3) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	
x ₁ ^(s) x ₁	x ₁
0.0000 0.0000	0.001571
0.1599 0.1597	0.001541
0.2887 0.2883	0.001476
0.5182 0.5175	0.001280
0.6157 0.6150	0.001163
0.7059 0.7052	0.001041
0.8693 0.8686	0.000784
0.9328 0.9322	0.000685
1.0000 0.9994	0.000585
AUXILIAF	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed	(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
in amber glass bottles and allowed to equilibrate for several days at constant	(3) 99+ %, anhydrous, Aldrich Chemical
temperature. Attainment of equilibrium was verified by several repetitive	Company.
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5$ % (relative error).

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COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) n-Octane; C ₈ H ₁₈ ; [111-65-9]	ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Acree, W.E., Jr. J. Chem. Eng. Data <u>1994</u> , 39, 114-116.
(3) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EIPERIMENTAL VALUES ^a t = 25.0 °C	
x3 ^(s) x3	×1
0.0000 0.0000	0.001838
0.1724 0.1721	0.001783
0.3201 0.3196	0.001658
0.5408 0.5400	0.001412
0.6384 0.6376	0.001263
0.7265 0.7257	0.001111
0.8791 0.8784	0.000826
0.9353 0.9346	0.000717
1.0000 0.9994	0.000585
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed	(2) 99+ %, anhydrous, Aldrich Chemical Company.
in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5$ % (relative error).

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Acree, W.E., Jr.
(2) Cyclohexane; C ₆ H ₁	2; [110-82-7]	I Char Fra Data 1994 29 114-116
(3) 2-Butanol; C ₄ H ₁₀ O	; [15892-23-6]	J. Chem. Eng. Data <u>1994</u> , 39, 114-116.
VARIABLES:		PREPARED BY:
T/K = 298, Solvent co	omposition	W.E. Acree, Jr.
1		
EXPERIMENTAL VALUES ^a t = 25.0 °C		
x3 ^(S)	*3	×1
0.0000	0.000	0.001553
0.1266	0.1264	0.001618
0.2285	0.2281	0.001565
0.4422	0.4416	0.001370
0.5429	0.5422	0.001247
0.6425	0.6418	0.001088
0.8210	0.8203	0.000829
0.9089	0.9083	0.000699
1.0000	0.9994	0.000585
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROC	CEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature thermometer, and an u spectrophotometer.	bath, calorimetric iltraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtu	res were prepared by	(2) HPLC Grade, 99.9+ %, Aldrich Chemical
in amber glass bottle	es and solvent placed	(2) 001 a setudore bland the standard
temperature. Attain	nent of equilibrium	(3) 99+ %, annydrous, Aldrich Chemical Company.
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
Concentrations determ metrically at 356 nm.	nined spectrophoto-	
		ESTIMATED ERRORS:
		T/K: ± 0.05.
		$x_3^{(3)}: \pm 0.0001.$ $x_1: \pm 1.5$ % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) Methylcyclohexane; C ₇ H ₁₄ ; (108-87-2)	J. Chem. Eng. Data 1994, 39, 114-116.
(3) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	
x, ^(s) x ₁	<i>x</i> ,
0.0000 0.0000	
0.1460 0.1457	0.001725
0.2585 0.2581	0.001647
0.4740 0.4733	0.001413
0.5832 0.5825	0.001262
0.5743 0.5735	0.001117
0.8541 0.8534	0.000821
0.0334 0.0334	0.000821
1,0000	0.000705
AU:	XILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimet thermometer, and an ultraviolet/visil spectrophotometer. Binary solvent mixtures were prepare weight. Excess solute and solvent pl in amber glass bottles and allowed t equilibrate for several days at cons temperature. Attainment of equilibr was verified by several repetitive measurements and by approaching equi brium from supersaturation. Aliquots saturated solutions transferred thro a coarse filter into tared volumetri flasks, weighed and diluted with met Concentrations determined spectropho metrically at 356 nm.	<pre>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 Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS: T/K; ± 0.05. x₃^(S): ± 0.0001. x₁: ± 1.5 % (relative error).</pre>

		1
COMPONENTS: (1) Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Acree, W.E., Jr.
 (2) 2,2,4-Trimet [540-84-1] (3) 2-Butanol; C 	hylpentane; C ₈ H ₁₈ ; 4H ₁₀ 0; [15892-23-6]	J. Chem. Eng. Data <u>1994</u> , 39, 114-116.
VARIABLES:		PREPARED BY:
T/K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	ES ^a	ļ
x3 ^(s)	×3	×1
0.0000	0.0000	0.001074
0.1574	0.1572	0.001116
0.3118	0.3115	0.001091
0.5396	0.5391	0.001000
0.6365	0.6359	0.000935
0.7292	0.7286	0.000863
0.8766	0.8760	0.000720
0.9475	0.9469	0.000646
1.0000	0.9994	0.000585
	AUXILIARY	INFORMATION
ETHOD: APPARATUS	/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ture bath, calorimetric an ultraviolet/visible r.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess so in amber glass b	ixtures were prepared by olute and solvent placed ottles and allowed to	(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
equilibrate for temperature. At was verified by	several days at constant tainment of equilibrium several repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
saturated solution a coarse filter flasks, weighed Concentrations do metrically at 35	saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. etermined spectrophoto- 6 nm.	molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.5 %$ (relative error).

COMP	ONENTS:		ORIGINAL MEASUREMENTS:
(1)	Anthracene; C ₁₄ H ₁₀	; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2)	t-Butylcyclohexan [3178-22-1]	ne; C ₁₀ H ₂₀ ;	J. Chem. Eng. Data <u>1994</u> , 39, 117-118.
(3)	2-Butanol; C ₄ H ₁₀ O;	[15892-23-6]	
VARI	ABLES:		PREPARED BY:
T/K	t = 298, Solvent co	omposition	W.E. Acree, Jr.
EXPE	RIMENTAL VALUES ^a 25.0 °C		
	x ₃ ^(s)	<i>x</i> ₃	x1
l	0.0000	0.0000	0.001978
	0.1795	0.1791	0.001977
	0.3264	0.3258	0.001833
	0.5520	0.5512	0.001513
	0.6528	0.6519	0.001343
	0.7394	0.7385	0.001167
	0.8794	0.8786	0.000854
	0.9348	0.9341	0.000735
	1.0000	0.9994	0.000585
		AUXILIARY	INFORMATION
MET	HOD: APPARATUS/PRO	OCEDURE	SOURCE AND PURITY OF MATERIALS:
Co th sp	ermometer, and an ectrophotometer.	e bath, calorimetric ultraviolet/visible	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bi we in eq te wa me br sa	nary solvent mixtu eight. Excess solut amber glass bottl uilibrate for seve imperature. Attain is verified by seve easurements and by ium from supersatu turated solutions	ares were prepared by the and solvent placed les and allowed to aral days at constant mment of equilibrium aral repetitive approaching equili- iration. Aliquots of transferred through	 (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.
a fl Cc me	coarse filter int asks, weighed and oncentrations deter strically at 356 n	diluted with methanol. mined spectrophoto- m.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

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COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2) n-Hexane; C ₆ 1	H ₁₄ ; [110-54-3]	T Chom Eng Data 1994 24 541-542
(3) 2-Methyl-1-p [78-83-1]	ropanol; C ₄ H ₁₀ O;	J. Chem. Eng. Data <u>1994</u> , 33, 341-343.
VARIABLES:		PREPARED BY:
T/K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU t = 25.0 °C	ES ^a	
x3 ^(s)	x3	×1
0.0000	0.0000	0.001274
0.1473	0.1471	0.001299
0.2688	0.2685	0.001236
0.4807	0.4802	0.001063
0.5889	0.5883	0.000947
0.6846	0.6840	0.000838
0.8524	0.8519	0.000645
0.9250	0.9245	0.000560
1.0000	0.9995	0.000470
	AUXILIARY	INFORMATION
METHOD: APPARATUS	S/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	uture bath, calorimetric l an ultraviolet/visible pr.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m	ixtures were prepared by	(2) 99+ mole %, Aldrich Chemical Company.
in amber glass b equilibrate for	solute and solvent placed sottles and allowed to several days at constant	(3) 99+ %, anhydrous, Aldrich Chemical Company.
temperature. At was verified by measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35	tainment of equilibrium several repetitive l by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. letermined spectrophoto- 66 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3 %$ (relative error).

COMPO	DNENTS:		ORIGINAL MEASUREMENTS:
(1)	Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2)	n-Heptane; C	C7H ₁₆ ; [142-82-5]	I Chan Eng Data 1994 20 541-543
(3)	2-Methyl-1-p	propanol; C ₄ H ₁₀ O;	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
	[/0-03 1]		
VARI	ABLES:		PREPARED BY:
T/K	= 298, Solve	ent composition	W.E. Acree, Jr.
EXPE t =	RIMENTAL VALU 25.0 °C	JES ^a	
	x3 ^(s)	*3	x1
	0.0000	0.000	0.001571
	0.1644	0.1642	0.001514
	0.2825	0.2821	0.001435
	0.5123	0.5117	0.001181
	0.6094	0.6088	0.001031
	0.7105	0.7099	0.000899
	0.8567	0.8561	0.000680
	0.9294	0.9289	0.000575
	1.0000	0.9995	0.000470
		AUXILIARY	INFORMATION
METH	HOD: APPARATU	IS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Con the spe	nstant temper ermometer, an ectrophotomet	ature bath, calorimetric d an ultraviolet/visible er.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bin we: in	ary solvent ight. Excess	mixtures were prepared by solute and solvent placed bottles and allowed to	(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
equ ter	uilibrate for nperature. A	several days at constant Attainment of equilibrium	(3) 99+ %, anhydrous, Aldrich Chemical Company.
mei bri sat fli Coi met	asurements an Lum from supe turated solut coarse filter asks, weighed ncentrations trically at (d by approaching equili- ersaturation. Aliquots of tions transferred through into tared volumetric and diluted with methanol. determined spectrophoto- 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
			ESTIMATED ERRORS:
			$T/K: \pm 0.05. x_3^{(s)}: \pm 0.0001. x_1: \pm 1.3 \ (relative error).$

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2) n-Octane; C ₈	H ₁₈ ; [111-65-9]	
(3) 2-Methyl-1-p [78-83-1]	propanol; C ₄ H ₁₀ O;	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
VARIABLES:		PREPARED BY:
T/K = 298, Solve	ent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUE $t = 25.0$ °C	IES ^a	
x ₃ (s)	x3	x1
0.0000	0.0000	0.001838
0.1786	0.1783	0.001742
0.3077	0.3072	0.001601
0.5373	0.5366	0.001278
0.6371	0.6364	0.001111
0.7281	0.7274	0.000955
0.8741	0.8735	0.000693
0.9385	0.9380	0.000581
1.0000	0.9995	0.000470
	AUXILIARY	INFORMATION
METHOD: APPARATUS	S/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ature bath, calorimetric an ultraviolet/visible er.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess s in amber glass h equilibrate for	nixtures were prepared by solute and solvent placed pottles and allowed to geveral days at constant	 (2) 99+ %, anhydrous, Aldrich Chemical Company. (3) 99+ % anhydrous, Aldrich Chemical
temperature. At was verified by measurements and	tainment of equilibrium several repetitive by approaching equili-	Company. Components 2 and 3 were stored over
brium from super saturated soluti a coarse filter flasks, weighed Concentrations of metrically at 35	saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. letermined spectrophoto- 66 nm.	molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3$ % (relative error).

COMPO	DNENTS:		ORIGINAL MEASUREMENTS:
(1)	Anthracene: C. H.	[120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2)	Cyclohexane; C,H.,	; [110-82-7]	-
(3)	2-Methyl-1-propan	ol; C ₄ H ₁₀ O;	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
	[78-83-1]		
VARI	ABLES:		PREPARED BY:
т/к	= 298, Solvent com	mposition	W.E. Acree, Jr.
EXPE t =	RIMENTAL VALUES ^a 25.0 °C		
	x ₃ ^(s)	<i>x</i> 3	x ₁
	0.0000	0.0000	0.001553
	0.1267	0.1265	0.001565
	0.2262	0.2259	0.001488
	0.4297	0.4292	0.001232
	0.5441	0.5435	0.001073
	0.6400	0.6394	0.000928
	0.8155	0.8149	0.000692
	0.9131	0.9126	0.000575
	1.0000	0.9995	0.000470
		AUXILIARY	INFORMATION
MET	HOD: APPARATUS/PROG	CEDURE	SOURCE AND PURITY OF MATERIALS:
Co: the sp	nstant temperature ermometer, and an u ectrophotometer.	bath, calorimetric ultraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bi	nary solvent mixtu ight. Excess solute	res were prepared by and solvent placed	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
in eq	amber glass bottle uilibrate for seven mperature. Attain	es and allowed to ral days at constant ment of equilibrium	 (3) 99+ %, anhydrous, Aldrich Chemical (3) Company
wa	s verified by seven	ral repetitive approaching equili-	Company.
br sa a fl Co me	ium from supersatu turated solutions coarse filter into asks, weighed and ncentrations deter trically at 356 nm	ration. Aliquets of transferred through tared volumetric diluted with methanol. mined spectrophoto-	molecular sieves and distilled shortly before use.
			ESTIMATED ERRORS:
			$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3 $ % (relative error).

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COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2) Methylcycloh [108-87-2]	exane; C ₇ H ₁₄ ;	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
(3) 2-Methyl-l-p [78-83-1]	ropanol; C ₄ H ₁₀ O;	
VARIABLES:		PREPARED BY:
<i>T</i> /K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	res ^a	
x, ^(s)	x3	x 1
0.0000	0.0000	0.001649
0.1438	0.1436	0.001697
0.2568	0.2564	0.001568
0.4769	0.4763	0.001265
0.5837	0.5831	0.001100
0.6739	0.6733	0.000963
0.8428	0.8422	0.000693
0.9143	0.9138	0.000590
1.0000	0.9995	0.000470
	AUXILIARY	INFORMATION
METHOD: APPARATUS	S/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ature bath, calorimetric an ultraviolet/visible ar.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess s	aixtures were prepared by solute and solvent placed	<pre>(2) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
equilibrate for temperature. At	several days at constant tainment of equilibrium	<pre>(3) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35	by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. determined spectrophoto- 56 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3$ % (relative error).

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
<pre>(3) 2-Methy1-1-propanol; C₄H₁₀O; [78-83-1]</pre>	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a $t = 25.0 ^{\circ}C$	
x ₁ ^(s) x ₁	x ₁
0.0000 0.0000	0.001074
0.1859 0.1857	0.001087
0.3227 0.3224	0.001019
0.5402 0.5397	0.000880
0.6451 0.6446	0.000805
0.7334 0.7329	0.000730
0.8780 0.8775	0.000591
0.9413 0.9408	0.000536
1.0000 0.9995	0.000470
AUXILIAR	Y INFORMATION
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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	 (2) HPLC Grade, 99.7 %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Company.
weasurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_{3}^{(5)}: \pm 0.0001.$ $x_{1}: \pm 1.3$ % (relative error).

	ORIGINAL MEASUREMENTS:
(1) Determine C W (120-12-7)	Zvajazne A I · Wolfe J · Acree W F Jr
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]	LValg2ne, A.I., Wolle, U., Actee, W.L., U.
$(2) = SurvicyCronexane; C_{10}H_{20};$ (3178-22-1)	J. Chem. Eng. Data <u>1994</u> , 39, 541-543.
(3) 2-Methyl-1-propanol; C ₄ H ₁₀ O; [78-83-1]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	
x ³ (2) x ²	×1
0.0000 0.0000	0.001978
0.1860 0.1856	0.001892
0.3238 0.3232	0.001716
0.5548 0.5541	0.001336
0.6531 0.6523	0.001150
0.7351 0.7344	0.000990
0.8806 0.8800	0.000699
0.9449 0.9444	0.000574
1.0000 0.9995	0.000470
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99 %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS: T/K: ± 0.05. x₃(s): ± 0.0001. x₃(s): ± 1.3 % (relative error).



COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; (C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Hexane; C ₆ H	1 ₁₄ ; [110-54-3]	I Chem Fog Data in progg
(3) 3-Methyl-1-bu [123-51-3]	atanol; C ₅ H ₁₂ O;	J. Chem. Eng. Data, in press.
VARIABLES:		PREPARED BY:
T/K = 298, Solver	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALUE $t = 25.0$ °C	ES ^a	
x3 ^(s)	*3	x 1
0.0000	0.0000	0.001274
0.1275	0.1273	0.001341
0.2355	0.2352	0.001312
0.4384	0.4379	0.001221
0.5447	0.5441	0.001146
0.6401	0.6394	0.001064
0.8269	0.8262	0.000890
0.9115	0.9108	0.000813
1.0000	0.9993	0.000727
^a x ₃ ^(s) : init fraction so the ternary	ial mole fraction of Lubility of the solut solution.	binary solvent mixture; x_1 : mole e; x_3 : mole fraction of component 3 in

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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	 SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ mole %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_3^{(S)}: \pm 0.0001.$ $x_1: \pm 1.3$ % (relative error).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C _{1/H10} ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Heptane; (C ₇ H ₁₆ ; [142-82-5]	
(3) 3-Methyl-1-b	$putanol; C_5H_{12}O;$	J. Chem. Eng. Data, in press.
[123-51-3]		
VARIABLES:		PREPARED BY:
T/K = 298, Solve	ent composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	ues*	<u></u>
x3 ^(s)	x 3	×1
0.000	0.0000	0.001571
0.1431	0.1429	0.001554
0.2545	0.2541	0.001500
0.4751	0.4745	0.001337
0.5713	0.5706	0.001234
0.6681	0.6674	0.001128
0.8383	0.8375	0.000916
0.9151	0.9143	0.000823
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary	0.9143 0.9993 Tial mole fraction of binary lubility of the solute; x ₃ : r solution.	0.000823 0.000727 solvent mixture; x ₁ : mole mole fraction of component 3 in
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary	0.9143 0.9993 tial mole fraction of binary lubility of the solute; x ₃ : r solution.	0.000823 0.000727 solvent mixture; x ₁ : mole mole fraction of component 3 in
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary	0.9143 0.9993 Cial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY	0.000823 0.000727 solvent mixture; x ₁ : mole mole fraction of component 3 in INFORMATION
0.9151 1.0000 ^a x3 ^(s) : init fraction so the ternary the ternary METHOD: APPARATU	0.9143 0.9993 tial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE	0.000823 0.000727 solvent mixture; x ₁ : mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS:
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary METHOD: APPARATU: Constant temper. thermometer, and spectrophotomet	0.9143 0.9993 tial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er.	0.000823 0.000727 solvent mixture; x ₁ : mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemica Company, Milwaukee, Wisconsin, USA, used as received.
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary METHOD: APPARATU: Constant temperathermometer, any spectrophotometor Binary solvent response	0.9143 0.9993 tial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er. mixtures were prepared by solute and solvent placed	0.000823 0.000727 solvent mixture; x ₁ : mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemica Company, Milwaukee, Wisconsin, USA, used as received. (2) HPLC Grade, 99.7+ %, Aldrich Chemica Company.
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary METHOD: APPARATU: Constant temperathermometer, and spectrophotomet Binary solvent models in amber glass in amber glass equilibrate for temperature. A	0.9143 0.9993 tial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er. mixtures were prepared by solute and solvent placed bottles and allowed to several days at constant ttainment of equilibrium	<pre>0.000823 0.000727 solvent mixture; x₁: mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemica Company, Milwaukee, Wisconsin, USA, used as received. (2) HPLC Grade, 99.7+ %, Aldrich Chemica Company. (3) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary METHOD: APPARATU Constant temper. thermometer, and spectrophotomet Binary solvent i weight. Excess in amber glass equilibrate for temperature. A was verified by measurements and brium from supe	0.9143 0.9993 Stial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er. mixtures were prepared by solute and solvent placed bottles and allowed to several days at constant ttainment of equilibrium several repetitive d by approaching equili- rsaturation. Aliquots of ions transformed theorem	 0.000823 0.000727 solvent mixture; x₁: mole mole fraction of component 3 in TINFORMATION SOURCE AND PURITY OF MATERIALS: Gold Label, 99.9+ %, Aldrich Chemica Company, Milwaukee, Wisconsin, USA, used as received. HPLC Grade, 99.7+ %, Aldrich Chemica Company. 99+ %, anhydrous, Aldrich Chemical Company. Source and 3 were stored over molecular sieves and distilled short before upo
0.9151 1.0000 ^a x ₃ ^(s) : init fraction so the ternary METHOD: APPARATU: Constant temper thermometer, and spectrophotomet Binary solvent weight. Excess in amber glass equilibrate for temperature. A was verified by measurements and brium from supe saturated solut a coarse filter flasks, weighed Concentrations of metrically at 3	0.9143 0.9993 Stial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er. mixtures were prepared by solute and solvent placed bottles and allowed to several days at constant ttainment of equilibrium several repetitive d by approaching equili- rsaturation. Aliquots of ions transferred through into tared volumetric and diluted with methanol. determined spectrophoto- 56 nm.	 0.000823 0.000727 solvent mixture; x₁: mole mole fraction of component 3 in TINFORMATION SOURCE AND PURITY OF MATERIALS: Gold Label, 99.9+ %, Aldrich Chemica Company, Milwaukee, Wisconsin, USA, used as received. HPLC Grade, 99.7+ %, Aldrich Chemica Company. 99+ %, anhydrous, Aldrich Chemical Company. Gomponents 2 and 3 were stored over molecular sieves and distilled short before use.
0.9151 1.0000 a x ₃ (s): init fraction so the ternary METHOD: APPARATU: Constant temperation spectrophotomet Binary solvent a weight. Excess in amber glass equilibrate for temperature. A was verified by measurements and brium from supe saturated solut a coarse filter flasks, weighed Concentrations of metrically at 3	0.9143 0.9993 Stial mole fraction of binary lubility of the solute; x ₃ : r solution. AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er. mixtures were prepared by solute and solvent placed bottles and allowed to several days at constant ttainment of equilibrium several repetitive d by approaching equili- rsaturation. Aliquots of ions transferred through into tared volumetric and diluted with methanol. determined spectrophoto- 56 nm.	 0.000823 0.000727 solvent mixture; x₁: mole mole fraction of component 3 in TINFORMATION SOURCE AND PURITY OF MATERIALS: Gold Label, 99.9+ %, Aldrich Chemica Company, Milwaukee, Wisconsin, USA, used as received. HPLC Grade, 99.7+ %, Aldrich Chemica Company. HPLC Grade, 99.7+ %, Aldrich Chemical Company. 99+ %, anhydrous, Aldrich Chemical Company. Somponents 2 and 3 were stored over molecular sieves and distilled short before use. ESTIMATED ERRORS:

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COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄	H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Octane; C ₈ H ₁₈ ;	; [111-65-9]	Tother Pro Data da mara
(3) 3-Methyl-1-buta [123-51-3]	anol; C ₅ H ₁₂ O;	J. Chem. Eng. Data, in press.
VARIABLES:		PREPARED BY:
T/K = 298, Solvent	composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ³ t = 25.0 °C		
x ₃ ^(s)	x ₃	x,
0.0000	0.0000	0.001838
0.1537	0.1534	0.001814
0.2672	0.2667	0.001728
0.4914	0.4907	0.001488
0.5939	0.5931	0.001345
0.6958	0.6950	0.001199
0.8537	0.8529	0.000952
0.9265	0.9257	0.000844
1.0000	0.9993	0.000727
	AUXILIARY	INFORMATION
METHOD: APPARATUS/P	ROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperatu thermometer, and a spectrophotometer.	re bath, calorimetric n ultraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mix weight. Excess sol in amber glass bot	tures were prepared by ute and solvent placed tles and allowed to	(2) 99+ %, anhydrous, Aldrich Chemical Company.
equilibrate for se temperature. Atta was verified by se	veral days at constant inment of equilibrium veral repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
measurements and b brium from supersa saturated solution a coarse filter in flasks, weighed an Concentrations det metrically at 356	by approaching equili- ituration. Aliquots of as transferred through ito tared volumetric ad diluted with methanol. ermined spectrophoto- nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3 $ (relative error).

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COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) Cyclohexane;	C ₆ H ₁₂ ; [110-82-7]	
(3) 3-Methyl-1-b	utanol; C ₅ H ₁₂ O;	J. Chem. Eng. Data, in press.
[123-51-3]		
VARIABLES:		PREPARED BY:
T/K = 298, Solve	nt composition	W.E. Acree, Jr.
EXPERIMENTAL VALU	'ES ^a	
x ₁ (\$)	<i>x</i> 3	x ₁
0.0000	0.0000	0.001553
0.1048	0.1046	0.001607
0.2011	0.2008	0.001561
0,3923	0.3918	0.001389
0-4977	0.4971	0.001277
0,5993	0.5986	0.001153
0.7958	0.7951	0.000934
0,8896	0.8889	0.000836
1,0000	0,9993	0.000727
	AUXILIARY	INFORMATION
METHOD: APPARATUS	/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotomete	ture bath, calorimetric an ultraviolet/visible r.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent m weight. Excess s	ixtures were prepared by olute and solvent placed	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
equilibrate for temperature. At	several days at constant tainment of equilibrium several repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
measurements and brium from super saturated soluti a coarse filter flasks, weighed Concentrations d metrically at 35	by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. letermined spectrophoto- 6 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3$ % (relative error).

COMP	onents:		ORIGINAL MEASUREMENTS:
(1)	Anthracene; C ₁₄ H ₁₀	₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2)	Methylcyclohexand [108-87-2]	e; C ₇ H ₁₄ ;	J. Chem. Eng. Data, in press.
(3)	3-Methyl-l-butand [123-51-3]	ol; C ₅ H ₁₂ O;	
VARI	ABLES:		PREPARED BY:
T/K	= 298, Solvent co	omposition	W.E. Acree, Jr.
EXPE	RIMENTAL VALUES ^a 25.0 °C		
	x ₁ ^(S)	Xz	X1
	0.0000	0.0000	0.001649
	0.1290	0.1288	0.001709
	0.2350	0.2346	0.001633
	0.4367	0.4361	0.001422
	0.5422	0.5415	0.001299
	0.6437	0.6430	0.001153
	0.8247	0.8239	0.000923
	0.9137	0.9129	0.000821
	1.0000	0.9993	0.000727
		AUXILIARY	INFORMATION
MET	HOD: APPARATUS/PRO	OCEDURE	SOURCE AND PURITY OF MATERIALS:
Co: the spe	nstant temperature ermometer, and an ectrophotometer.	e bath, calorimetric ultraviolet/visible	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bi we in	nary solvent mixtu ight. Excess solut amber glass bottl	ares were prepared by te and solvent placed les and allowed to	(2) 99+ %, anhydrous, Aldrich Chemical Company.
ter wa me	mperature. Attair s verified by seve asurements and by	ament of equilibrium aral repetitive approaching equili-	(3) 99+ %, anhydrous, Aldrich Chemical Company. Components 2 and 3 were stored over
br sa fl Co me	ium from supersatu turated solutions coarse filter into asks, weighed and incentrations deter strically at 356 no	uration. Aliquots of transferred through o tared volumetric diluted with methanol. rmined spectrophoto- m.	molecular sieves and distilled shortly before use.
			ESTIMATED ERRORS:
			$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3$ % (relative error).

Components :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	J. Chem. Eng. Data, in press.
(3) 3-Methyl-1-butanol; C ₅ H ₁₂ O; [123-51-3]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ⁸ t = 25.0 °C	
x ₃ ^(s) x ₃	x ₁
0.0000 0.0000	0.001074
0.1476 0.1474	0.001114
0.2838 0.2835	0.001103
0.4998 0.4993	0.001042
0.6038 0.6032	0.000990
0.6973 0.6966	0.000937
0.8537 0.8530	0.000831
0.9196 0.9189	0.000782
1.0000 0.9993	0.000727
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to	 (2) HPLC Grade, 99.7 %, Aldrich Chemical Company. (2) Obstantiation of the state of
temperature. Attainment of equilibrium	Company.
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1.3 $ (relative error).

MPONENTS:	ORIGINAL MEASUREMENTS:
1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
<pre>2) t-Butylcyclohexane; C₁₀H₂₀; [3178-22-1]</pre>	J. Chem. Eng. Data, in press.
3) 3-Methyl-1-butanol; C ₅ H ₁₂ O; [123-51-3]	
NRIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
CPERIMENTAL VALUES ^a	
x, ^(s) x ₃	x ₁
0.0000 0.0000	0.001978
0.1685 0.1682	0.001938
0.2866 0.2861	0.001843
0.5168 0.5160	0.001545
	0,001400
0.7070	0.001217
0.7072 0.7083	0.000944
0.8650 0.8642	0.000953
0.9274 0.9266	0.000852
-	
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol Concentrations determined spectrophoto- metrically at 356 nm.	 (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: $T/K: \pm 0.05.$ $x_{3}^{(s)}: \pm 0.0001.$ $x_{1}: \pm 1.3 $ (relative error).

(1) Anthracene; C		ORIGINAL MEASUREMENIS:
	: ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
(2) n-Hexane; C ₆ H	14; [110-54-3]	S.A.
(3) 1-Octanol; C ₈	H ₁₈ 0; [111-87-5]	Fluid Phabe Equilibr. <u>1994</u> , 92, 233-253.
VARIABLES:		PREPARED BY:
<i>T</i> /K = 298, Solver	it composition	W.E. Acree, Jr.
EXPERIMENTAL VALUE	2S ^a	I
x _z ^(S)	x,	<i>x</i> ,
0.0000	0.0000	0.001274
0.0774	0.0773	0.001469
0.1758	0.1755	0.001608
0.3536	0.3530	0.001827
0.4524	0.4515	0.001917
0.5528	0.5517	0.001979
0.7728	0.7712	0.002101
0.8747	0.8728	0.002138
1 0000	0.9978	0.002160
,	solution.	
	Solution.	
	AUXILIARY	INFORMATION
METHOD: APPARATUS/	AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD: APPARATUS/ Constant temperat thermometer, and spectrophotometer	AUXILIARY /PROCEDURE cure bath, calorimetric an ultraviolet/visible	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
METHOD: APPARATUS/ Constant temperat thermometer, and spectrophotometer Binary solvent mi	AUXILIARY PROCEDURE Sure bath, calorimetric an ultraviolet/visible 	INFORMATION 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.
METHOD: APPARATUS/ Constant temperat thermometer, and spectrophotometer Binary solvent mi weight. Excess so in amber glass bo equilibrate for a	AUXILIARY /PROCEDURE ture bath, calorimetric an ultraviolet/visible 	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ mole %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
METHOD: APPARATUS/ Constant temperat thermometer, and spectrophotometer Binary solvent mi weight. Excess so in amber glass bo equilibrate for s temperature. At was verified by s measurements and brium from supers saturated solutio a coarse filter i flasks, weighed a Concentrations de metrically at 356	AUXILIARY /PROCEDURE ture bath, calorimetric an ultraviolet/visible tures were prepared by blute and solvent placed bottles and allowed to several days at constant tainment of equilibrium several repetitive by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. termined spectrophoto- in m.	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ mole %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use.</pre>
METHOD: APPARATUS/ Constant temperati thermometer, and spectrophotometer Binary solvent mi weight. Excess so equilibrate for s temperature. Att was verified by s measurements and brium from supers saturated solution a coarse filter i flasks, weighed a Concentrations de metrically at 356	AUXILIARY PROCEDURE ture bath, calorimetric an ultraviolet/visible to an ultraviolet/visible to and solvent placed bottles and allowed to several days at constant tainment of equilibrium several repetitive by approaching equili- saturation. Aliquots of ons transferred through into tared volumetric and diluted with methanol. termined spectrophoto- onm.	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ mole %, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS:</pre>

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COMPONENTS: (1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) n-Heptane; C ₇ H ₁₆ ; [142-82-5] (3) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]	ORIGINAL MEASUREMENTS: Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, A.I. Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
VARIABLES: T/K = 298, Solvent composition	PREPARED BY: W.E. Acree, Jr.
EXPERIMENTAL VALUES^a t = 25.0 °C	
a_3 a_3 0.0000 0.0000 0.1018 0.1016 0.1925 0.1921 0.3897 0.3889 0.4808 0.4798 0.5865 0.5853 0.7841 0.7824 0.8958 0.8939 1.0000 0.9978 $a_{x_3}^{(s)}$: initial mole fraction of binar fraction solubility of the solute; x_3 the ternary solution.	0.001571 0.001738 0.001835 0.002002 0.002057 0.002098 0.002135 0.002163 0.002160 ry solvent mixture; x ₁ : mole : mole fraction of component 3 in
AUXILIA	RY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
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 equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flages weighed and diluted with methanol	 (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.

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COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C	14 ^H 10; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
(2) n-Octane; C ₈ H	₈ ; [111-65-9]	Fluid Dhage Fauilibr 1994 92, 233-253
(3) 1-Octanol; C ₈ H	i ₁₈ 0; [111-87-5]	1111 1 mase Equilibr. <u>1774</u> , 72, 205 200.
1		
VARIABLES:		PREPARED BY:
T/K = 298, Solven	t composition	W.E. Acree, Jr.
EXPERIMENTAL VALUE t = 25.0 °C	S ^a	
x3 ⁽⁸⁾	×3	x 1
0.0000	0.0000	0.001838
0.1090	0.1088	0.001948
0.2110	0.2106	0.002040
0.4021	0.4012	0.002138
0.5071	0.5060	0.002169
0.6139	0.6126	0.002182
0.8015	0.7998	0.002175
0.9021	0.9001	0.002167
1.0000	0.9978	0.002160
	AUXILIARY	INFORMATION
METHOD: APPARATUS/	PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperat thermometer, and spectrophotometer Binary solvent min weight. Excess so in amber glass bo equilibrate for s temperature. Atta was verified by s measurements and i brium from supers saturated solution a coarse filter i flasks, weighed an Concentrations de metrically at 356	ure bath, calorimetric an ultraviolet/visible xtures were prepared by lute and solvent placed ttles and allowed to everal days at constant ainment of equilibrium everal repetitive by approaching equili- aturation. Aliquots of ns transferred through nto tared volumetric nd diluted with methanol. termined spectrophoto- nm.	 (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 ⁽⁶⁾ : ± 0.0001. x ₁ : ± 1.5 % (relative error).
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Compo	nents :		ORIGINAL MEASUREMENTS:
(1)	Anthracene; C ₁₄ H ₁₀	; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.
(2)	Cyclohexane; C ₆ H ₁₂	; [110-82-7]	Fluid Phase Equilibr. 1994, 92, 233-253.
(3)	1-Octanol; C ₈ H ₁₈ O;	[111-87-5]	
VARIA	ABLES:		PREPARED BY:
T/K	= 298, Solvent co	mposition	W.E. Acree, Jr.
EXPEI t =	RIMENTAL VALUES ^a 25.0 °C		
	x3 ^(s)	*3	x ₁
	0.0000	0.000	0.001553
	0.0815	0.0814	0.001730
	0.1521	0.1518	0.001804
	0.3128	0.3122	0.001937
	0.4106	0.4098	0.002002
	0.5153	0.5142	0.002048
	0.7254	0.7239	0.002120
	0.8499	0.8481	0.002143
	1.0000	0.9978	0.002160
		AUXILIARY	INFORMATION
METH	HOD: APPARATUS/PRO	CEDURE	SOURCE AND PURITY OF MATERIALS:
Con the spe	nstant temperature ermometer, and an ectrophotometer.	bath, calorimetric ultraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bin	nary solvent mixtu	res were prepared by	(2) HPLC Grade, 99.9+ %, Aldrich Chemical
in equ	amber glass bottl uilibrate for seve	es and allowed to ral days at constant	(3) 99+ %, anhydrous, Aldrich Chemical
wat	s verified by seve asurements and by	approaching equili-	Components 2 and 3 years should sugge
br sa a fl Co me	ium from supersatu turated solutions coarse filter into asks, weighed and ncentrations deter trically at 356 nm	ration. Aliquots of transferred through tared volumetric diluted with methanol. mined spectrophoto- n.	molecular sieves and distilled shortly before use.
{			ESTIMATED ERRORS:
			$T/K: \pm 0.05.$
			$x_3^{(s)}$: ± 0.0001 . x_1 : ± 1.5 % (relative error)

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [12	20-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.
<pre>(2) Methylcyclohexane; C7F [108-87-2]</pre>	I ₁₄ ;	Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
(3) 1-Octanol; C ₈ H ₁₈ O; [11	1-87-5]	
VARIABLES:		PREPARED BY:
T/K = 298, Solvent compos.	ition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C		
x3 ^(s) x3		×1
0.0000 0.00	000	0.001649
0.0884 0.08	382	0.001885
0.1712 0.17	709	0.001966
0.3497 0.34	190	0.002058
0.4438 0.44	129	0.002090
0.5454 0.54	142	0.002119
0.7623 0.70	507	0.002147
0.8752 0.8	733	0.002154
1.0000 0.99	978	0.002160
the ternary solution.		
	AUXILIARY	INFORMATION
METEOD: APPARATUS/PROCEDURI	5	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and an ultray spectrophotometer. Binary solvent mixtures we weight. Excess solute and in amber glass bottles and equilibrate for several di temperature. Attainment of was verified by several ro measurements and by appro- brium from supersaturation saturated solutions trans; a coarse filter into tared flasks, weighed and dilute Concentrations determined metrically at 356 nm.	calorimetric violet/visible ere prepared by solvent placed d allowed to ays at constant of equilibrium of equilibrium aching equili- n. Aliquots of ferred through d volumetric ed with methanol. spectrophoto-	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) 99+ %, anhydrous, Aldrich Chemical Company. (3) 99+ %, anhydrous, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS: T/K: ± 0.05. x ₃ (s): ± 0.0001. x ₁ : ± 1.5 % (relative error).

MPONENTS :		ORIGINAL MEASUREMENTS:
1) Anthracene; (C _{1/H10} ; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker,
2) 2,2,4-Trimet	hylpentane; C ₈ H ₁₈ ;	S.A.
[540-84-1]		riula Phase Equilibr. <u>1994</u> , 92, 233-253.
(3) 1-Octanol; C_g	₃ H ₁₈ O; [111-87-5]	
ARIABLES:		PREPARED BY:
r/K = 298, Solve:	nt composition	W.E. Acree, Jr.
EXAMPLE 1 In the second sec	ESª	
x ₇ ^(s)	x ₃	x ₁
0.0000	0.0000	0.001074
0.1236	0.1234	0.001261
0.2128	0.2125	0.001378
0.4069	0.4062	0.001608
0.5092	0.5083	0.001719
0.6123	0.6112	0.001809
0.8054	0.8038	0.001987
0.8992	0.8973	0.002065
1.0000	0.9978	0.000160
a _{x3} (s): init fraction sol the ternary	tial mole fraction of binary lubility of the solute; x_3 : solution.	solvent mixture; x ₁ : mole mole fraction of component 3 in
<pre>* x₃(\$): init fraction so the ternary</pre>	tial mole fraction of binary lubility of the solute; x3: solution.	solvent mixture; x ₁ : mole mole fraction of component 3 in
<pre>* x₃(\$): init fraction so the ternary</pre>	tial mole fraction of binary lubility of the solute; x3: 1 solution.	solvent mixture; x ₁ : mole mole fraction of component 3 in TINFORMATION
<pre>* x₃(\$): init fraction so the ternary METHOD: APPARATU</pre>	Lial mole fraction of binary lubility of the solute; x3: solution. AUXILIARY SS/PROCEDURE	solvent mixture; x ₁ : mole mole fraction of component 3 in r INFORMATION SOURCE AND PURITY OF MATERIALS:
 x₃^(s): init fraction sol the ternary METEOD: APPARATU Constant temper thermometer, an spectrophotomet 	Lial mole fraction of binary lubility of the solute; x3: solution. AUXILIARY SS/PROCEDURE rature bath, calorimetric d an ultraviolet/visible ser.	Solvent mixture; x ₁ : mole mole fraction of component 3 in INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
 * x₃⁽⁵⁾: init fraction sol the ternary METHOD: APPARATU Constant temper thermometer, an spectrophotomet Binary solvent weight. Excess in amber class 	AUXILIARY AUXILIARY Solution. AUXILIARY AUXILI	<pre>Solvent mixture; x₁: mole mole fraction of component 3 in 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.</pre>
 * x₃⁽⁵⁾: init fraction sol the ternary METHOD: APPARATU Constant temper thermometer, an spectrophotomet Binary solvent weight. Excess in amber glass equilibrate for temperature. A 	AUXILIARY AUXILIARY S/PROCEDURE ature bath, calorimetric d an ultraviolet/visible er. mixtures were prepared by solute and solvent placed bottles and allowed to several days at constant ttainment of equilibrium c several apporting	<pre>Solvent mixture; x₁: mole mole fraction of component 3 in SOURCE AND FURITY 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.</pre>
 * x₃⁽⁵⁾: init fraction sol the ternary METHOD: APPARATU Constant temper thermometer, an spectrophotomet Binary solvent weight. Excess in amber glass equilibrate for temperature. A was verified by measurements an brium from supe saturated solut a coarse filter flasks, weighed Concentrations metrically at 3 	AUXILIARY AUXILIARY Solution. AUXILIARY AUXILIARY AUXILIARY SAMPACEDURE Fature bath, calorimetric dd an ultraviolet/visible ter. mixtures were prepared by solute and solvent placed bottles and allowed to several repetitive dby approaching equili- resturation. Aliquots of the stand and allowed to is several repetitive dby approaching equili- resturation. Aliquots of the stand spectrophoto- diant diluted with methanol. determined spectrophoto- 356 nm.	<pre>Solvent mixture; x₁: mole mole fraction of component 3 in 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. (3) 99+ %, anhydrous, Aldrich Chemical Company. Components 2 and 3 were stored over molecular sieves and distilled shortly before use.</pre>
 * x₃⁽⁵⁾: init fraction sol the ternary METHOD: APPARATU Constant temper thermometer, an spectrophotomet Binary solvent weight. Excess in amber glass equilibrate for temperature. A was verified by measurements an brium from supe saturated solut a coarse filter flasks, weighed Concentrations metrically at 3 	AUXILIARY AUXILIARY Solution. AUXILIARY Solution. AUXILIARY SS/PROCEDURE Fature bath, calorimetric dd an ultraviolet/visible fer. mixtures were prepared by solute and solvent placed bottles and allowed to solute and solvent placed bottles and allowed to is several days at constant ttainment of equilibrium reseveral repetitive dd by approaching equili- fresturation. Aliquots of clons transferred through into tared volumetric and diluted with methanol. determined spectrophoto- 356 nm.	 Solvent mixture; x₁: mole mole fraction of component 3 in SOURCE AND PURITY OF MATERIALS: Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. HPLC Grade, 99.7 %, Aldrich Chemical Company. 99+ %, anhydrous, Aldrich Chemical Company. 99+ %, anhydrous, Aldrich Chemical Company. Gomponents 2 and 3 were stored over molecular sieves and distilled shortly before use. ESTIMATED ERRORS:

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COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1)	(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Zvaigzne, A.I.; Acree, W.E., Jr.	
(2)	(2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1]		J. Chem. Eng. Data <u>1994</u> , 39, 117-118.	
(3)	1-Octanol; C ₈ H ₁₈ O	; [111-87-5]		
VARIABLES:			PREPARED BY:	
T/K = 298, Solvent composition			W.E. Acree, Jr.	
EXPER t =	IMENTAL VALUES ^a 25.0 °C			
	x ₃ ^(s)	x3	×1	
	0.0000	0.0000	0.001978	
	0.1124	0.1122	0.002151	
	0.2170	0.2165	0.002198	
	0.4191	0.4181	0.002274	
	0.5221	0.5209	0.002274	
	0.6185	0.6171	0.002249	
	0.8152	0.8134	0.002219	
	0.9127	0.9107	0.002180	
	1.0000	0.9978	0.002160	
AUXILIARY INFORMATION				
METHO	D: APPARATUS/PROC	CEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.			(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber class bottles and allowed to			(2) 99 %, Aldrich Chemical Company.	
equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive			(3) 99+ %, anhydrous, Aldrich Chemical Company.	
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.			Components 2 and 3 were stored over molecular sieves and distilled shortly before use.	
			ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_{3}^{(3)}: \pm 0.0001.$ $x_{1}: \pm 1$ % (relative error).	
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COMPONENTS :		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Acree, W.E., Jr.; Zvaigzne, A.I.		
(2) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]		Fluid Phase Fouilibr in pross		
(3) 1-Propanol; C ₃ H ₈ (0; [71-23-8]	Tiul Phase Squiibit, in press.		
VARIABLES:		PREPARED BY:		
T/K = 298, Solvent o	composition	W.E. Acree, Jr.		
EIPERIMENTAL VALUES ^a $t = 25.0 ^{\circ}C$				
x3 ^(s)	x3	x ₁		
0.0000	0.000	0.000801		
0.1331	0.1330	0.000783		
0.2419	0.2417	0.000762		
0.4468	0.4465	0.000716		
0.5538	0.5534	0.000692		
0.6472	0.6468	0.000674		
0.8289	0.8284	0.000631		
0.9043	0.9037	0.000616		
1.0000	0.9994	0.000591		
AUXILIARY INFORMATION				
METHOD: APPARATUS/PR	OCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperatur thermometer, and an spectrophotometer.	e bath, calorimetric ultraviolet/visible	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 		
Binary solvent mixt	ures were prepared by	(2) HPLC Grade, 99.8+ %, Aldrich Chemical		
in amber glass bott equilibrate for sev temperature. Attai	les and allowed to eral days at constant nment of equilibrium	Company. (3) 99+ %, anhydrous, Aldrich Chemical Company.		
was verified by sev measurements and by brium from supersat saturated solutions a coarse filter int flasks, weighed and Concentrations dete metrically at 356 m	eral repetitive approaching equili- uration. Aliquots of transferred through to tared volumetric diluted with methanol. rmined spectrophoto- um.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.		
		ESTIMATED ERRORS:		
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).		
	OPTATNAL MEASUREMENTS .			
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(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	ACLES, W.L., Jr.; 2valgzne, A.I.			
(2) 2-Butanol; $C_4H_{10}O;$ [15892-23-6]	Fluid Phase Equilibr., in press.			
(3) 1-propanol; C_3H_80 ; [71-23-8]				
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,			
0.0000 0.0000	0.000585			
0.1310 0.1309	0.000586			
0.2470 0.2469	0.000584			
0.4461 0.4458	0.000586			
0.5495 0.5492	0.000586			
0.6514 0.6510	0.000588			
0.8243 0.8238	0.000593			
0.9065 0.9060	0.000592			
1.0000 0.9994	0.000591			
AUXILIAR	Y INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.			
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed	(2) 99+ %, anhydrous, Aldrich Chemical Company.			
in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium	(3) 99+ %, anhydrous, Aldrich Chemical Company.			
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.			
	ESTIMATED ERRORS:			
	$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).			

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Components :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Acree, W.E., Jr.; Zvaigzne, A.I.
(2) 2-Propanol; C ₃ H ₈ O; [67-63-0]		Fluid Phase Equilibr., in press.
(3) 1-Propanol; C ₃ H ₈ O; [71-23-8]		
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALU	ES ^a	
x ₁ (s)	x 3	x1
0.0000	0.0000	0.000411
0.1092	0.1092	0.000436
0.2068	0.2067	0.000449
0.4016	0.4014	0.000478
0.5073	0.5070	0.000497
0.6105	0.6102	0.000516
0.7955	0.7951	0.000553
0.8882	0.8877	0.000572
1.0000	0.9994	0.000591
	AUXILIARY	INFORMATION
METHOD: APPARATU	S/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant tempera thermometer, and spectrophotometer	ature bath, calorimetric d an ultraviolet/visible er.	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent weight. Excess in amber glass	mixtures were prepared by solute and solvent placed bottles and allowed to	<pre>(2) 99+ %, anhydrous, Aldrich Chemical Company.</pre>
equilibrate for temperature. A was verified by	several days at constant ttainment of equilibrium several repetitive	(3) 99+ %, anhydrous, Aldrich Chemical Company.
measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		T/K: \pm 0.05. $x_3^{(s)}$: \pm 0.0001. x_1 : \pm 1 % (relative error).

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.
(2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]	Fluid Phase Equilibre in press
(3) 1-Propanol; C ₃ H ₈ O; [71-23-8]	Tidid Flase Equilibri, in press.
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C	
x ₁ ^(s) x ₃	<i>x</i> ₁
0.0000 0.0000	0.002160
0.2116 0.2112	0.001873
0.3583 0.3577	0.001655
0.5747 0.5739	0.001322
0.6793 0.6785	0.001145
0.7689 0.7681	0.000996
0.8921 0.8914	0.000782
0.9481 0.9474	0.000688
1.0000 0.9994	0.000591
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	 (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were prepared by weight. Excess solute and solvent placed	(2) 99+ %, anhydrous, Aldrich Chemical Company.
in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium	(3) 99+ %, anhydrous, Aldrich Chemical Company.
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.	Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1$ % (relative error).

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Acree, W.E., Jr.; Zvaigzne, A.I.
(2) 1-Butanol; $C_2H_{10}O$; [71-36-3]		Fluid Dhage Fouiliby is succe
(3) 2-Propanol; C ₃ H ₈ O; [67-63-0	ן ס	Fluid Phase Equilibr., in press.
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a $t = 25.0 ^{\circ}C$		
x ₃ ^(s) x ₃		x ₁
0.0000 0.0000		0.000801
0.1362 0.1361		0.000757
0.2456 0.2454		0.000710
0.4369 0.4366		0.000630
0.5448 0.5445		0.000584
0.6427 0.6423		0.000548
0.8193 0.8189		0.000482
0.9061 0.9057		0.000449
1.0000 0.9996		0.000411
the ternary Bolution.		
	AUXILIARY	INFORMATION
METROD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, cal thermometer, and an ultraviol spectrophotometer.	lorimetric et/visible	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtures were p weight. Excess solute and solv in amber class bottles and all	prepared by vent placed lowed to	(2) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
equilibrate for several days a temperature. Attainment of e	at constant guilibrium	(3) 99+ %, anhydrous, Aldrich Chemical Company.
was verified by several repet measurements and by approaching	itive ng equili-	Components 2 and 3 were stored over
brium from supersaturation. Aliquits of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		T/K: + 0.05.
		$x_3^{(s)}$: + 0.0001. x: + 1 % (relative error).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Acree, W.E., Jr.; Zvaigzne, A.I.
(2) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6]		
(3) 2-Propanol; C ₃ H ₈ O;	[67-63-0]	Fluid Phase Equilibr., in press.
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C		
x3 ^(s)	x3	×1
0.0000	0.0000	0.000585
0.1355	0.1354	0.000564
0.2441	0.2440	0.000545
0.4403	0.4401	0.000512
0.5429	0.5426	0.000495
0.6486	0.6483	0.000476
0.8169	0.8165	0.000445
0.9008	0.9004	0.000430
1.0000	0.9996	0.000411
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature thermometer, and an u spectrophotometer.	bath, calorimetric ltraviolet/visible	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Binary solvent mixtur weight. Excess solute	es were prepared by and solvent placed	(2) 99+ %, anhydrous, Aldrich Chemical Company.
in amber glass bottle equilibrate for sever temperature. Attainm	s and allowed to al days at constant ent of equilibrium	 (3) 99+ %, anhydrous, Aldrich Chemical Company.
was verified by several repetitive measurements and by approaching equili- brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		Components 2 and 3 were stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_3^{(s)}: \pm 0.0001.$ $x_1: \pm 1 $ (relative error).

COMPONENTS:			ORIGINAL MEASUREMENTS;
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		; [120-12-7]	Acree, W.E., Jr.; Zvaigzne, A.I.
(2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]		[111-87-5]	Fluid Phase Equilibres in press.
(3)	2-Butanol; C ₄ H ₁₀ O;	[15892-23-6]	riulu rhase squiitsit, in piess.
VARIABLES:			PREPARED BY:
T/K = 298, Solvent composition		mposition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 25.0 °C			
	x3 ^(s)	x3	x 1
	0.0000	0.0000	0.002160
	0.1773	0.1770	0.001911
	0.3041	0.3036	0.001698
	0.5351	0.5344	0,001314
	0 6329	0 6321	0.001164
	0.0328	0.8321	0.001013
ĺ	0.7235	0.7228	0.001012
	0.8703	0.8696	0.000787
1	0.9308	0.9302	0,000696
	1.0000	0.9994	0.000585
the ternary Bolution.			
		AUXILIARY	INFORMATION
METE	IOD: APPARATUS/PROC	CEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		bath, calorimetric ltraviolet/visible	 Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Bir	nary solvent mixtur	es were prepared by	(2) 99+ %, anhydrous, Aldrich Chemical
wei in	ight. Excess solute amber glass bottle	e and solvent placed es and allowed to	Company.
equ ten	uilibrate for seven nperature. Attainn	al days at constant nent of equilibrium	(3) 99+ %, anhydrous, Aldrich Chemical Company.
was	s verified by sever asurements and by a	al repetitive	Components 2 and 3 were stored over
brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 356 nm.		ation. Aliquots of transferred through tared volumetric diluted with methanol. nined spectrophoto-	molecular sieves and distilled shortly before use.
			ESTIMATED ERRORS:
			T/K: + 0.05.
			$x_{3}^{(s)}: \pm 0.0001.$ $x_{1}: \pm 1$ % (relative error).

(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	
	Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V. Valkoucky, S.W.
(2) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Fruizon Sai Tachnol 1990 24 639-646
(3) Water; H ₂ O; [7732-18-5]	$\frac{1}{2}$
	a private communication.)
VARIABLES:	PREPARED BY:
T/K = 296, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a	1
φ ₁ ^(s) C ₁ /	(mol dm ⁻³)
0.00 4.3	L6 x 10 ⁻⁷
0-10 1-1	30×10^{-6}
0.20 7.4	16×10^{-6}
0.30	33 × 10 ⁻⁵
0.40	24×10^{-4}
0.50	
AUXILIAR)	INFORMATION
AUXILIAR) METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
AUXILIARS METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an HPLC equipped with	SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in the paper.
AUXILIAR) METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.	SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in the paper. (2) Purity and chemical source were not
AUXILIARY METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection. Binary solvent mixtures were prepared by volume. Excess solute and solvent placed	 INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in the paper. (2) Purity and chemical source were not specified in the paper.
AUXILIARS METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection. Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solu- tions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile- methanolswater mobile phase were word in	 SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in the paper. (2) Purity and chemical source were not specified in the paper. (3) Purity and chemical source were not specified in the paper.
AUXILIARS METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection. Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solu- tions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile- methanol-water mobile phase were used in the chromatographic analysis.	 INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in the paper. (2) Purity and chemical source were not specified in the paper. (3) Purity and chemical source were not specified in the paper.
AUXILIARS METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection. Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solu- tions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile- methanol-water mobile phase were used in the chromatographic analysis.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in the paper. (2) Purity and chemical source were not specified in the paper. (3) Purity and chemical source were not specified in the paper.</pre>

Components:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.: Yalkowsky, S.H.
(2) Methanol; CH ₄ O; [67-56-1]	Environ, Sci. Technol, 1990, 24, 639-646
(3) Water; H ₂ O; [7732-18-5]	(Numerical values obtained from L.S. Lee in
	a private communication.)
VARIABLES:	PREPARED BY:
T/K = 296, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a t = 23.0 °C	
$\phi_2^{(s)}$ $c_1/($	(mol dm ⁻³)
0.00 4.1	6 x 10 ⁻⁷
0.10 7.4	1 x 10 ⁻⁷
0.20 1.1	7 x 10 ⁻⁶
0.30 2.8	8 x 10 ⁻⁶
0.40 1.0	2 × 10 ⁻⁵
0.50 4.3	4 x 10 ⁻⁵
0.60 1.1	2×10^{-4}
0.80 1.0	3 x 10 ⁻³
0.90 2.2	8 x 10 ⁻³
1.00 4.8	2×10^{-3}
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.	 Purity and chemical source were not specified in the paper.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed	(2) Purity and chemical source were not specified in the paper.
in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con-	(3) Purity and chemical source were not specified in the paper.
stant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for	
tions were analyzed by reversed-phase	
detection. Excitation and emission	
respectively. An octadecylsilanized	
methanol-water mobile phase were used in	
the chromatographic analysis.	ESTIMATED ERRORS:
	$T/K_{1} \pm 1$
	φ_2 : \pm 0.01 (compiler). C_1 : \pm 5 % (relative error; compiler).

Components:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.: Yalkowsky, S.H.
(2) 2-Propanol; C ₃ H ₈ O; [67-63-0]	Environ. Sci. Technol. 1990, 24, 639-646.
(3) Water; H ₂ O; [7732-18-5]	(Numerical values obtained from L.S. Lee in a private communication.)
VARIABLES:	PREPARED BY:
T/K = 296, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a $t = 23.0 ^{\circ}C$	
$\phi_2^{(s)}$ $c_1/($	mol dm ⁻³)
0.00 4.16	5 × 10 ⁻⁷
0.10 7.69	9 x 10 ⁻⁷
0.20 4.57	/ x 10 ⁻⁶
0.30 2.47	7 x 10 ⁻⁵
0.40 1.03	3 x 10 ⁻⁴
0.50 5.49	9 x 10 ⁻⁴
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection. Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con- stant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solu- tions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acctonitrile- methanol-water mobile phase were used in the chromatographic analysis.	 (1) Purity and chemical source were not specified in the paper. (2) Purity and chemical source were not specified in the paper. (3) Purity and chemical source were not specified in the paper. ESTIMATED ERRORS: T/K: ± 1. φ₂(s): ± 0.01 (compiler). c₁: ± 5 % (relative error; compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Dimethyl sulfoxide; C₂H₆OS; [67-68-5] Environ. Sci. Technol. 1990, 24, 639-646. (Numerical values obtained from L.S. Lee in (3) Water; H₂O; [7732-18-5] a private communication.) VARIABLES: PREPARED BY: T/K = 296, Solvent composition W.E. Acree, Jr. **EXPERIMENTAL VALUES^a** t = 23.0 °C $\phi_2^{(s)}$ $c_1/(\text{mol } \text{dm}^{-3})$ 4.16 x 10^{-7} 0.00 6.06 x 10⁻⁷ 0.10 2.29×10^{-6} 0.20 0.30 6.73 x 10⁻⁶ 2.10×10^{-5} 0.40 5.89×10^{-5} 0.50 2.13 x 10⁻⁴ 0.60 8.86 x 10⁻⁴ 0.70 3.76×10^{-3} 0.80 1.35×10^{-2} 0.90 4.23×10^{-2} 1.00 ^a $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1 : molar solubility (mol dm⁻³) of the solute. AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric (1) Purity and chemical source were not thermometer, and an HPLC equipped with fluorescence detection. specified in the paper. (2) Purity and chemical source were not Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a con-stant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant soluspecified in the paper. (3) Purity and chemical source were not specified in the paper. tions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile-methanol-water mobile phase were used in the chromatographic analysis. ESTIMATED ERRORS:

T/K: ± 1 . $\phi_2^{(s)}$: ± 0.01 (compiler). c_1 : ± 5 % (relative error; compiler).

BENZ[a]ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

n-heptane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons
- D. <u>Esters</u>
- E. <u>Ethers</u>
- F. <u>Haloalkanes_and Haloaromatic Hydrocarbons</u>
- G. <u>Alcohols</u>
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benz[a]anthracene; C ₁₈ H ₁₂ ;	Lissi, E.A.; Abuin, E.B.
[56-55-3] (2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	-
$t/^{\circ}C$ $c_{1}/(mol dm^{-3})$	
20.0 0.0	133
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, centrifuge, thermometer, and an uv/visible spectro- photometer.	 Purity not given, commercial sample of unspecified source, was used as received.
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the mea- sured absorbance using the Beer-Lambert law.	(2) Purity and chemical source not given, purification procedure not specified.
	ESTIMATED ERRORS:
	$T/K: \pm 2.$ $c_1:$ unknown.

BENZO(b)FLUORENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

- A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>
- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons
- D. <u>Esters</u>
- E. Ethers
- F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>
- G. Alcohols

1-octanol

- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Benzo[b]fluorene; C₁₇H₁₂; [243-17-4] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. <i>Environ. Sci. Technol.</i> <u>1985</u> , <i>19</i> , 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$t/^{\circ}C$ $c_1/(mol dm^{-3})$	
25.0 0.03	1563
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection.	(1) Highest available commercial purity, specific chemical supplier not given, was used as received.
Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 %	(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
SE30 ultraphase column.	ESTIMATED ERRORS:
	T/K: \pm 0.1 (compiler). c ₁ : \pm 3 % (relative error; compiler).

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BENZO[ghi]PERYLENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

n-heptane cyclohexane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

methylbenzene

D. <u>Seters</u>

ethyl butyrate

- E. Ethere
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. Alcohols
- H. Ketones

acetone cyclohexanone acetophenone

- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[ghi]perylene; C ₂₂ H ₁₂ ;	Lissi, E.A.; Abuin, E.B.
(2) n-Heptane; $C_7 H_{16}$; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C C1/	mol dm ⁻³)
20.0 0.0	512
	THROPHERTON
AUTILIARI	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the mea- sured fluorescence emission intensity.	(2) Purity and chemical source not given, purification procedure not specified.
	ESTIMATED ERRORS:
	$T/K: \pm 2.$ $C_1: unknown.$

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Benzo[ghi]perylene; C ₂₂ H ₁₂ ; [191-24-2] (2) Cucloberane: C H : (110-82-7)	Carre, O.R.; Phillips, D.J.; Brennecke, J.F.		
(2) cyclonexane, C_{n12} , $[110-52-7]$	Ind. Eng. Chem. Res. <u>1994</u> , 33, 1255–1262.		
VARIABLES:	PREPARED BY:		
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.		
EIPERIMENTAL VALUES			
t/°C x ₂	x 1		
21.0 0.9999	0.000149		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Ultraviolet/visible spectrophotometer and centrifugal automatic particle anal- yzer.	 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer. 		
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) HPLC Grade, 99+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.		
Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.	ESTIMATED ERRORS:		
	T/K: ± 2 (Compiler). x_1 : ± 9.5 % (relative error).		

COMPONENTS	ORIGINAL MEASUREMENTS:		
<pre>(1) Benzo[ghi]perylene; C₂₂H₁₂; [191-24-2] (2) Methylbenzene; C₇H₈; [108-88-3]</pre>	Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. <u>1994</u> , 33, 1355-1362.		
VARIABLES:	PREPARED BY:		
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	<i>x</i> 1		
21.0 0.9980	0.00204		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:			
Ultraviolet/visible spectrophotometer and centrifugal automatic particle anal- yzer.	 (1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer. 		
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) ACS Grade, 99 %, Fisher Scientific, Pittaburgh, Pennsylvania, USA, was used as received.		
Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.	ESTIMATED ERRORS: $T/K: \pm 2$ (Compiler). $x_1: \pm 1.4$ % (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Benzo[ghi]perylene; C₂₂H₁₂; [191-24-2] (2) Ethyl butyrate; C,H₁O₂; [105-54-4]</pre>	Carre, O.R.; Phillips, D.J.; Brennecke, J.F.		
	Ind. Eng. Chem. Res. <u>1994</u> , 33, 1355-1362.		
VARIABLES:	PREPARED BY:		
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	x ₁		
21.0 0.9988	0.00116		
AUXILIARY INFORMATION			
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Ultraviolet/visible spectrophotometer and centrifugal automatic particle anal- yzer.	(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.		
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) 99 %, Aldrich Chemical Company, was used as received.		
Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.	ESTIMATED ERRORS: $T/K: \pm 2$ (Compiler). $x_1: \pm 6.5$ % (relative error).		

COMPONENTS :	ORIGINAL MEASUREMENTS: Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. <u>1994</u> , 33, 1355-1362.		
<pre>(1) Benzo[ghi]perylene; C₂₂H₁₂;</pre>			
(2) Acetone; C ₃ H ₆ O; [67-64-1]			
VARIABLES:	PREPARED BY:		
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	x 1		
21.0 0.9994	0.000634		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Ultraviolet/visible spectrophotometer and centrifugal automatic particle anal- yzer.	(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.		
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) ACS Grade, 99.5 %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.		
Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.	ESTIMATED ERRORS:		
	T/K: ± 2 (Compiler). x ₁ : ± 0.7 % (relative error).		

ORIGINAL MEASUREMENTS:			
Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. <u>1994</u> , 33, 1255-1262.			
PREPARED BY:			
W.E. Acree, Jr.			
×1			
0.00400			
AUXILIARY INFORMATION			
SOURCE AND PURITY OF MATERIALS:			
 (1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer. 			
(2) 99.8 %, Aldrich Chemical Company, was used as received.			
ESTIMATED ERRORS: T/K: ± 2 (Compiler). x1: ± 5.1 % (relative error).			

COMPONENTS	OPTOTNAL MEASIDEMENTS.		
<pre>(1) Benzo[ghi]perylene; C₂₂H₁₂; [191-24-2] (2) Acetophenone; C₈H₈O; [98-86-2]</pre>	ORIGINAL MEASUREMENTS: Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. <u>1994</u> , 33, 1355-1362.		
VARIABLES:	PREPARED BY:		
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	x 1		
21.0 0.9936	0.00640		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Ultraviolet/visible spectrophotometer and centrifugal automatic particle anal- yzer.	 (1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer. 		
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and the solvent evaporated. Residue dissolved in cyclohexane and	(2) 99 %, Aldrich Chemical Company, was used as received.		
diluted quantitatively for spectrophoto- metric analysis. Attainement of equili- brium was verified by repetitive measure- ments after 24 hour intervals.	ESTIMATED ERRORS: $T/K: \pm 2$ (Compiler). $x_1: \pm 4.6$ % (relative error).		

BENZO[a]PYRENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

n-heptane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene

- D. <u>Esters</u>
- E. <u>Ethers</u>
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. <u>Alcohols</u>
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8]	Lissi, E.A.; Abuin, E.B.		
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.		
VARIABLES:	PREPARED BY:		
T/K = 293	W.E. Acree, Jr.		
EIPERIMENTAL VALUES			
t/°C C ₁ /	(mol dm ⁻³)		
20.0 0.0034			
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifu- gation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming	(2) Purity and chemical source not given, purification procedure not specified.		
that the dilute solution behavior extra- polates up to saturation point.	ESTIMATED ERRORS:		
	$T/K: \pm 2.$ $c_1:$ unknown.		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8]	Mishra, D.S.; Yalkowsky, S.H.		
(2) Benzene; C ₆ H ₆ ; [71-43-2]	Ind. Eng. Chem. Res., <u>1990</u> , 29, 2278-2283.		
VARIABLES:	PREPARED BY:		
<i>T/</i> K = 296	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	x ₁		
23.0 0.9646	0.0354		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, rotator, thermometer, and an uv/visible spectro- photometer.	 Reagent grade, source not specified, was used as received. 		
Excess solute and solvent placed in screw-capped test tube and allowed to equilibrate for 3 days with gentle agita- tion in a constant temperature bath. Samples centrifuged for 30 minutes and concentrations were determined spectro- photometrically. Attainment of equili- brium verified by repetitive measurements	(2) Reagent grade, source not specified, was used as received.		
4 days later.	ESTIMATED ERRORS:		
	T/K: \pm 0.1 (compiler). x_1 : \pm 5 % (relative error; compiler).		

BIPHENYL SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

- A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>
 - n-hexane n-heptane n-octane tetracosane octacosane cyclohexane methylcyclohexane cis-1,2-dimethylcyclohexane trans-1,2-dimethylcyclohexane trans-1,4-dimethylcyclohexane cis-1,4-dimethylcyclohexane cis-1,3-dimethylcyclohexane decahydronaphthalene
- B. Alkenes
- C. Aromatic Hydrocarbons

benzene
methylbenzene
ethylbenzene
naphthalene
2-methylnaphthalene
2,6-dimethylnaphthalene
1,2-diphenylethane
1,2,3,4-tetrahydronaphthalene

- D. Esters
- E. Ethers

1,4-dioxane diphenyl ether

F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>

dichloromethane trichloromethane 1,2-dibromoethane 1,1-dichloroethane 1,2-dichloroethane chlorobenzene 1,4-dichlorobenzene hexafluorobenzene

G. <u>Alcohols</u>

1-octanol 1-octadecanol H. Ketones

benzophenone

I. <u>Miscellaneous Pure Solvents</u>

carbon disulfide pyridine thiophene indole diphenylamine nitrobenzene 1-octadecanoic acid

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C _{12^H10} ; [92-52-4]	Acree, W.E., Jr.			
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	Int. J. Pharm. <u>1984</u> , 18, 47-52.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EIPERIMENTAL VALUES				
t/°C x ₂	*1			
25.0 0.8767	0.1233			
AUXILIARY INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo-	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.			
hexane. Concentrations determined spectrophotometrically at 250 nm.	ESTIMATED ERRORS:			
	T/K: \pm 0.05. x ₁ : \pm 1 % (relative error).			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/° c x ₂	x1
25.0 0.876	0.124
AUXILIARY	INFORMATION
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.
noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

COMPONENTS :		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]		Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. <u>1986</u> , 31, 225-230.			
VARIABLES:		PREPARED BY:			
T/K = 303, 308 and 313		W.E. Acree, Jr.			
EXPERIMENTAL V	ALUES				
t∕°C	x 2	x 1	t/° C	<i>x</i> 2	<i>x</i> 1
30.0	0.8392	0.1608	40.0	0.7369	0.2631
35.0	0.7994	0.2006			
		AUXILIARY	INFORMATIO	N	
METHOD: APPARA	TUS/PROCEDURE	8	SOURCE AND PURITY OF MATERIALS:		MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo- hexane. Concentrations determined spectrophotometrically at 250 nm.		(2) 99 % store tille	, Aldrich Che ed over molec ed shortly be	emical Company, was cular sieves and dis- efore use.	
		ESTIMATED $T/K: \pm 0$ $x_1: \pm 1$ %	ERRORS: .05. (relative e	error).	

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Acree, W.E., Jr.		
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Int. J. Pharm. <u>1984</u> , 18, 47-52.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	x ₁		
25.0 0.8619	0.1381		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo-	(2) 99+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.		
hexane. Concentrations determined spectrophotometrically at 250 nm.	ESTIMATED ERRORS:		
	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Warner, J.C.; Scheib, R.C.; Svirbely, W.J.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	J. Chem. Phys. <u>1934</u> , 2, 590-594.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
T/K ×2	x 1
299.7 0.860	0.140
308.4 0.784	0.216
313.1 0.726	0.274
316.3 0.665	0.335
319.9 0.591	0.409
322.2 0.532	0.468
322.3 0.525	0.475
328.5 0.335	0.665
330.7 0.284	0.726
332.7 0.197	0.803
333.7 0.194	0.806
334.8 0.164	0.836
335.7 0.143	0.857
337.2 0.108	0.892
339.2 0.066	0.934
341.3 0.028	0.972
UA	ILLIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a prec thermometer.	(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was
Solubilities were measured using a dynamic method. Mixtures of known co trations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gent rotation to thoroughly mix contents. temperature was slowly increased and bility visually determined by noting temperature at which the last trace solid solute disappeared. Measureme	hol. ncen- (2) Purity not specified, Eastman Kodak Company, was used as received. Bath solu- the of mts wits.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.002. (compiler).

	r			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Lissi, E.A.; Abuin, E.B.			
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.			
VARIABLES:	PREPARED BY:			
T/K = 293	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C c ₁ /((mol dm ⁻³)			
20.0 0.45				
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.			
Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifu- gation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming	(2) Purity and chemical source not given, purification procedure not specified.			
that the dilute solution behavior extra- polates up to saturation point.	ESTIMATED ERRORS:			
	$T/K: \pm 2.$			

COMPONENTS :		ORIGINAL MEASUREMENTS:				
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) n-Heptane; C₇H₁₆; [142-82-5]</pre>			Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. <u>1986</u> , 31, 225-230.			
VARIABLES:			PREPARED F	BY:		
T/K = 303, 30	8 and 313		W.E. Acre	ee, Jr.		
EXPERIMENTAL V	ALUES		•			
t/°C	x 2	×1	t/°C	x 2	x 1	
30.0	0.8250	0.1750	40.0	0.7227	0.2773	
35.0	0.7786	0.2214				
		AUXILIARY	INFORMATION	8		
METHOD: APPARA	TUS/PROCEDURI	E	SOURCE AND	D PURITY OF M	ATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.			(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a			(2) 99+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.			
urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo- hexane. Concentrations determined spectrophotometrically at 250 nm.			ESTIMATED $T/K: \pm 0$ $x_1: \pm 1$ %	ERRORS: .05. (relative e	rror).	

COMPONENTS:

Biphenyl; C₁₂H₁₀; [120-12-7]
 n-Heptane; C₇H₁₆; [110-54-3]

EVALUATOR:

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Denton, Texas 76203-5068 (USA)
June, 1994
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CRITICAL EVALUATION:

Biphenyl solubilities in n-heptane were retrieved from papers by Warner et al. (1), Acree et al. (2), Acree (3), Chang (4), and Lissi and Abuin (5). The first study reports observed values at several temperatures, Acree et al. determined values at 303, 308 and 313 K, and the latter three studies give the mole fraction solubility at either 298 K or 293 K. The value of Lissi was excluded from the critical evaluation since the n-heptane solvent was saturated with water, rather than a dried solvent.

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

 $Ln x_1 = -5153.7 (1/T) + 15.229 \qquad (r = 0.9982)$ for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.1279$, and differs by about 8 - 10 % from experimental values of $x_1 = 0.1381$ (3) and $x_1 = 0.138$ (4).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

1. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. J. Chem. Phys. 1934, 2, 590-594.

2. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.

3. Acree, W.E., Jr. Int. J. Pharm. 1984, 18, 47-52.

- 4. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.
- 5. Lissi, E.A.; Abuin, E.B. Bol Soc. Chil. Quin. 1981, 26, 19-34.

COMPONENTS :	ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.				
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).				
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EXPERIMENTAL VALUES	_				
t/°C x ₂	x ₁				
25.0 0.862	0.138				
AUXILIAR	LY INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.				
noting the temperature at which the last trace of solid solute disappeared. Sol-	ESTIMATED ERRORS:				
ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).				

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Acree, W.E., Jr.			
(2) n-Octane; C _g H ₁₈ ; [111-65-9]	Int. J. Pharm. <u>1984</u> , 18, 47-52.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂	×1			
25.0 0.8520	0.1480			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo-	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.			
hexane. Concentrations determined spectrophotometrically at 250 nm.	ESTIMATED ERRORS:			

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Biphenyl; C₁₂H₁₀; [92-52-4] Chang, W. (2) n-Octane; C₈H₁₈; [111-65-9] Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969). VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C *x*2 x₁ 0.853 0.147 25.0 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath and a precision (1) Purity, source and purification procethermometer. dures not specified. (2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by as received. noting the temperature at which the last trace of solid solute disappeared. Sol-ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus ESTIMATED ERRORS: T/K: precision \pm 0.1. $x_1: \pm 2$ % (relative error; compiler). $1/\bar{T}$ graph.

COMPONENTS:	ORIGINAL N	EASUREMENTS :			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-	Acree, W C.L.	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.			
(2) n-Octane; C ₈ H ₁₈ ; [111-	Int. J. I	Pharm. <u>1986</u> ,	31, 225-230.		
VARIABLES:	PREPARED H	3Y:			
T/K = 303, 308 and 313	W.E. Acre	ee, Jr.			
EXPERIMENTAL VALUES					
t/°C x ₂	×1	t/°C	x ₂	x 1	
30.0 0.8164	0.1836	40.0	0.7109	0.2891	
35.0 0.7707	0.2293				
	AUXILIARY	INFORMATION	Ĩ		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer, and an ultra- spectrophotometer.	(1) 99 %, Milwa lized	Aldrich Che uukee, Wiscon 1 3 times fro	mical Company, sin, USA, recrystal- m methanol.		
Excess solute and solvent glass bottles and allowed for several days at consta Attainment of equilibrium repetitive measurements. J urated solutions transfer	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.				
coarse filter into tared of flasks, weighed and dilute hexane. Concentrations de	ESTIMATED	ERRORS :			
spectrophotometrically at	$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).				

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COMPONEN	COMPONENTS :		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Vitali, G.				
(2) Tet:	(2) Tetracosane; C ₂₄ H ₅₀ ; [646-31-1]		Int. DATA Ser., Ser. A <u>1984</u> , 94.			
VARIABLE	5:			PREPARED BY:		
Tempera	ture			W.E. Acree, Jr.		
EXPERIMEN	TAL VALUES					
	T/K	*2	x 1	T/K	<i>x</i> 2	×1
	323.8	1.000	0.000	340.3	0.045	0.955
	323.4	0.980	0.020	340.8	0.044	0.956
	323.3	0.972	0.028	341.5	0.022	0.978
	322.8	0.942	0.058	341.9	0.012	0.988
	321.8	0.882	0.118	342.0	0.007	0+993
	320.6	0.804	0.196	342.3	0.000	1.000
	319.8	0.718	0.282			
	319.1	0.641	0.359			
	318.7	0.623	0.377			
	318.0	0.586	0.414			
	318.6	0.568	0.432			
	319.7	0.544	0.456			
	320.8	0.534	0.466			
	321.6	0.512	0.488			
	323.9	0.477	0.523			
	326.0	0.436	0.564			
	327.8	0.395	0.605			
	328.8	0.383	0.617			
	330.5	0.339	0.661			
	333.9	0.253	0.747			
	336.1	0.183	0.817			
	337.4	0.132	0.868			
	337.6	0.120	0.880			
	338.7	0.087	0.913			
	339.5	0.068	0.932			
			AUXILIARY	INFORMATION		<u> </u>
METHOD:	APPARATUS/P	ROCEDURE		SOURCE AND PURIT	Y OF MATERIA	LS:
Constant	t temperatu eter.	re bath and a	a precision	(1) 99 %, Ega, as received	Steinheim, C	Germany, was used
Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased Solubility determined by wirel		(2) 97 %, Baker was used as	, Deventer, received.	The Netherlands,		
noting t trace of	the tempera f solid solu	ture at which ite appeared	h the first	ESTIMATED ERRORS T/K: precision x_1 : \pm 0.001.	± 0.25.	

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Vitali, G.		
(2) Octacosane; C ₂₈ H ₅₈ ; [630-02-4]		Int. DATA Ser., Ser. A <u>1984</u> , 95.		
		DEEDADED BY.		
VARIABLES:		WE Acres. Jr.		
EXPERIMENTAL VALUES				
T/K	x 2	x 1		
334.7	1.000	0.000		
334.5	0.986	0.014		
334.3	0.971	0.029		
334.0	0.952	0.048		
333.5	0.922	0.078		
332.3	0.853	0.147		
331.0	0.767	0.233		
329.5	0.670	0.330		
329.0	0.585	0.415		
327.3	0.505	0.495		
326.2	0.460	0.540		
326.2	0.399	0.601		
331.1	0.306	0.694		
333.4	0.250	0.750		
335.7	0.187	0.813		
337.5	0.128	0.872		
339.9	0.072	0.928		
341.2	0.033	0.967		
341.4	0.023	0.977		
341.9	0.011	0.989		
342.1	0.003	0.997		
342.3	0.000	1.000		
METHOD: APPARATUS/PROCEDURE	AUTITIEKI	SOURCE AND PURITY OF MATERIALS,		
Constant temperature bath and a r	recision	(1) 99 %, Ega, Steinheim, Germany, was used		
thermometer.		as received.		
Mixtures of known concentrations in open containers and placed in	put constant	(2) 98 %, Ega, Steinheim, Germany, was used as received.		
temperature to equilibrate. Sampl were rocked while bath temperatur	es e slowly			
decreased. Solubility determined noting the temperature at which t	by visual the first	ESTIMATED ERRORS:		
trace of solid solute appeared.		T/K: precision + 0.25.		
		$x_1: \pm 0.001.$		

COMPONENTS:	<u> </u>	ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C ₁₂ H ₁₀ ; (92-52-4]	Acree, W.E., Jr.				
(2) Cyclohexane; C ₆ H ₁₂ ;	; [110-82-7]	Int. J. Pharm. <u>1984</u> , 18, 47-52.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°C	*2	<i>x</i> 1				
25.0	0.8079	0.1921				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature by thermometer, and an ul spectrophotometer.	ath, calorimetric traviolet/visible	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.				
Excess solute and solv glass bottles and allo for several days at co Attainment of equilibr repetitive measurement urated solutions trans coarse filter into tar flasks, weighed and di	vent placed in amber wed to equilibrate onstant temperature. fium verified by s. Aliquots of sat- oferred through a red volumetric luted with cyclo-	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.				
hexane. Concentration spectrophotometrically	ns determined at 250 nm.	ESTIMATED ERRORS:				
		$T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).				

COMPONENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]			ORIGINAL M	ORIGINAL MEASUREMENTS: Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data <u>1985</u> , 30, 403-409.			
			Choi, P.B McLaughli J. Chem.				
				v.			
Temperature		FREFRED B					
		W.E. Acre	e, Jr.				
EXPERIMENTAL V	ALUES						
T/K	*2	x 1	T/K	×2	×1		
302.35	0.7652	0.2348	326.95	0.3071	0.6929		
310.45	0.6460	0.3540	333.05	0.1748	0.8252		
314.65	0.5681	0.4319					
320.85	0.4384	0.5616					
		AUXILIAR	Y INFORMATION	1			
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS :		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly		(1) 99.6 Roche over lized (2) Gold Compa	 99.6 %, Eastman Kodak Chemical Company, Rochester, New York, USA, was passed over activated alumina and recrystal- lized from toluene Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received. 				
noting the te trace of soli	mperature at d solute dis	which the last appeared.	ESTIMATED	ERRORS:			
			T/K: prec	$T/K: precision \pm 0.1.$			

ORIGINAL MEASUREMENTS: COMPONENTS : (1) Biphenyl; C₁₂H₁₀; [92-52-4] Chang, W. (2) Cyclohexane; C₆H₁₂; [110-82-7] Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969). VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C **x**2 **x**1 25.0 0.810 0.190 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath and a precision (1) Purity, source and purification procethermometer. dures not specified. (2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Sol-ubilities at 298 K interpolated from ESTIMATED ERRORS: T/K: precision \pm 0.1. x₁: \pm 2 % (relative error; compiler). experimental values using $\ln x_1$ versus 1/T graph.

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		McLaughlin, E.; Zainal, H.A.				
(2) Cyclohexa	ane; C ₆ H ₁₂ ; [1]	10-82-7]	J. Chem.	Soc. <u>1960</u> ,	3854-3857.	
VARIABLES: Temperature		PREPARED BY: W.E. Acree, Jr.				
EXPERIMENTAL V	ALUES		ļ	······		
T/K	x ₂	×1	T/K	*2	x 1	
299.5	0.7987	0.2013	331.2	0.2186	0.7814	
310.4	0.6503	0.3497				
318.3	0.4978	0.5022				
325.2	0.3473	0.6527				
		AUXILIARY	INFORMATION	1		
METHOD: APPARA	TUS/PROCEDURE	5	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			 Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant. Purity, source and purification method was not specified. 			
trace of soli	mperature at .d solute disa	appeared.	ESTIMATED T/K: prec $x_1: \pm 0.00$	ision <u>+</u> 0.1. 003 (compile:	c).	

COMPONENTS:

- (1) Biphenyl; C₁₂H₁₀; [120-12-7]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]

EVALUATOR:

W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-506 June, 1994 76203-5068

(USA)

CRITICAL EVALUATION:

Biphenyl solubilities in cyclohexane were retrieved from papers by Choi et al. (1), McLaughlin and Zainal (2), Acree et al. (3), Acree (4) and Chang (5). The first two studies report observed values at several temperatures, Acree et al. determined values at 303, 308 and 313 K, and the latter two studies give the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the five studies from the critical evaluation.

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

Ln
$$x_1 = -4295.7 (1/T) + 12.770$$
 (r = 0.9975)
for variation of biphenyl solubility with absolute temperature (see graph below).
Back-calculated solubility at 298 K is $x_1 = 0.1944$, and differs by about 1 - 2 %
from experimental values of $x_1 = 0.1921$ (4) and $x_2 = 0.190$ (5).



Graphical plot of $Ln x_1$ versus 1/T

REFERENCES

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Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin J. Chem. Eng. Data 1985,
1.
      30, 403-409.
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McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 3854-3857. 2.

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з.
      Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.
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4.
      Acree, W.E., Jr. Int. J. Pharm. 1984, 18, 47-52.
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5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:		ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Acree, W C.L.	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.			
(2) Cyclones	kane; C6 ⁿ 12; [1.	10-82-7]	Int. J.	Pharm. <u>1986</u> ,	31, 225-230.	
VARIABLES:			PREPARED	BY:		
T/K = 303, 308 and 313			W.E. Acı	ee, Jr.		
EXPERIMENTAL	VALUES					
t/°C	x 2	x 1	t/°C	*2	x 1	
30.0	0.7529	0.2471	40.0	0.6052	0.3948	
35.0	0.6825	0.3175				
		AUXILIARY	INFORMATIC	N	·	
METHOD: APPAR	RATUS/PROCEDURI	3	SOURCE AN	D PURITY OF M	ATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.			(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat-			(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.			
repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo- hexane. Concentrations determined spectrophotometrically at 250 nm.		ESTIMATED $T/K: \pm 0$ $x_1: \pm 1$) ERRORS: 0.05. % (relative e	rror).		
			· ·			

COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.				
(2) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).				
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EXPERIMENTAL VALUES					
t/°C x ₂	×1				
25.0 0.817	0.183				
AUXILIARY INFORMATION					
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.				
noting the temperature at which the last trace of solid solute disappeared. Sol-	ESTIMATED ERRORS:				
ubilities at 298 K interpolated from	T/K: precision ± 0.1.				
experimental values using in x ₁ versus 1/T graph.	$x_1: \pm 2$ % (relative error; compiler).				
······					
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COMPONENTS :		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [9	92-52-4]	Chang, W. Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
(2) cis-1,2-Dimethylcy C ₈ H ₁₆ ; [2207-01-4]	clohexane;				
VARIABLES:		PREPARED BY:			
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	*2	×1			
25.0	0.805	0.195			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature be thermometer.	ath and a precision	 Purity, source and purification proce- dures not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.			
noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.		ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W. Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
(2) trans-1,2-Dimethylcyclohexane; C ₈ H ₁₆ ; [6876-23-9]				
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂	<i>x</i> 1			
25.0 0.817	0.183			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.			
noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).			

COMPONENTS	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W. Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
<pre>(2) trans-1,4-Dimethylcyclohexane; C₈H₁₆; [2207-04-7]</pre>				
VARIABLES:	PREPARED BY:			
<i>T/</i> K = 298	W.E. Acree, Jr.			
EIPERIMENTAL VALUES	-			
t/°C x ₂	<i>x</i> 1			
25.0 0.827	0.173			
AUXILIARY	INFORMATION .			
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.			
noting the temperature at which the last	ESTIMATED ERRORS:			
ubilities at 298 K interpolated from experimental values using ln x ₁ versus 1/T graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).			

CONPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [9	2-52-4]	Chang, W.			
(2) cis-1,4-Dimethylcyd	:lohexane;	Ph.D Dissertation, North Dakota State Uni-			
C ₈ H ₁₆ ; [624-29-3]	·	versity, North Dakota, USA (1969).			
VARIABLES:		PREPARED BY:			
m/x - 209					
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	x 2	x ₁			
25.0	0.818	0.182			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature ba thermometer.	th and a precision	 Purity, source and purification proce- dures not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from		(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.			
		ESTIMATED ERRORS:			
		T/K: precision + 0.1.			
experimental values usi 1/T graph.	$ng \ln x_1 versus$	x_1 : ± 2 % (relative error; compiler).			
		1			

COMPONENTS :		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [9	2-52-4]	Chang, W. Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969). PREPARED BY:			
(2) cis-1,3-Dimethylcyc C ₈ H ₁₆ ; [638-04-0]	:lohexane;				
VARIABLES:					
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	x2	x 1			
25.0	0.828	0.172			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bathermometer.	ath and a precision	 Purity, source and purification proce- dures not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus 1/T graph.		(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.			
		ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).			

COMPONENTS :		ORIG	INAL MEA	SUREMENT S:					
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Coor	1, J.E.;	Auwaerter,	J.E.;	McLaugh	ilin, E.		
(2)	Decahydrona [91-17-8]	phthalene;	с ₁₀ н ₁₈ ;	Flu	id Phase	Equilibr.	<u>1989</u> ,	44, 305	-345.
VARI	ABLES:			PREPA	ARED BY:				
Temperature		W.E.	Acree,	Jr.					
EXPE	RIMENTAL VAL	UES							
	T/K	*2	<i>x</i> 1	T/K		x 2	x 1		
	309.0	0.6389	0.3611	328	2	0.4477	0.738	35	
	316.0	0.5260	0.4740						
	318.2	0.4820	0.5180						
	324.3	0.3594	0.6406						
			AUXILIARY	INFORM	ATION				
METH	OD: APPARATU	S/PROCEDURE		SOURC	E AND P	URITY OF MA	TERIALS	5:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(1)	99.6 %, waukee, over an then re 99+ %, isomer trans,	Aldrich Ch Wisconsin, activated a crystallize Aldrich Che ratio of 60 stored over	emical USA, v alumina d from mical (.6 % ci molecu	Company vas pass a column solutic Company, is and 3 ilar sie	, Mil- ed and n. having 9.4 % eves.		
not tra	ing the temp ce of solid	erature at solute disa	which the last ppeared.	ESTIN T/K: X1:	ATED ER precis: + 0.0003	RORS: ion <u>+</u> 0.1.			

COMPONENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Benzene; C ₆ H ₆ ; [71-43-2]		ORIGINAL MEASUREMENTS: Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data <u>1985</u> , 30, 403-409.				
						VARIABLI
Temperature		W.E. Acree, Jr.				
EXPERIM	ENTAL VAL	UES				
T/1	к	*2	x 1	T/K	x 2	x 1
30'	7.95	0.5167	0.4833	328.95	0.2289	0.7711
31:	3.85	0.4439	0.5561	333.15	0.1578	0.8422
310	6.85	0.4068	0.5932			
323	3.65	0.3103	0.6897			
			AUXILIARY	INFORMATION		
METHOD:	APPARATU	S/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(1) 99.6 % Roches over a lized (2) Gold I Compar	Eastman K ster, New Yo activated al from toluen Label, 99.9+ ny, was used	odak Chemical Company, rk, USA, was passed umina and recrystal- e %, Aldrich Chemical as received.		
		ESTIMATED E T/K: preci $x_1: \pm 0.00$	ERRORS: ision <u>+</u> 0.1. 003.			

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.
(2) Benzene; C ₆ H ₆ ; [71-43-2]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	1
t/°C x ₂	<i>x</i> ₁
25.0 0.619	0.381
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Spectroanalyzed, Eastman Organic Chem- ical Company, USA, was used as received.
noting the temperature at which the last	ESTIMATED ERRORS:
ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Benzene; C ₆ H ₆ ; [71-43-2]		McLaughlin, E.; Zainal, H.A. <i>J. Chem. Soc</i> . <u>1959</u> , 863-867.			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	<i>x</i> 2	x 1			
310.2	0.4882	0.5118			
320.8	0.3522	0.6478			
332.4	0.1805	0.8195			
336.4	0.1084	0.8916			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDU	JRE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		 Purity not specified, Gesellschaft fur Teerverwertung, passed over an alumina column with benzene eluant. "AnalaR", was dried over sodium wire and freshly distilled before use. 			
		ESTIMATED ERRORS: T/K: precision <u>+</u> 0.1. x ₁ : <u>+</u> 0.0003 (compiler).			

COMPONENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		ORIGINAL MEASUREMENTS: Warner, J.C.; Scheib, R.C.; Svirbely, W.J.				
						(2) Benzene; (
VARIABLES:						
Temperature	Temperature		W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES					
T/K	*2	x 1	T/K	x 2	×1	
301.1	0.590	0.410	318.7	0.374	0.626	
316.3	0.415	0.585	322.6	0.323	0.677	
317.5	0.395	0.605	325.5	0.187	0.713	
		AUXILIARY	INFORMATION	4		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE ANT	PURITY OF N	MATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples upper protected upplies bath temperature slowly		(1) Purit Compa recry hol. (2) Thiop was c	y not specif any, Rocheste ystallized se phene free, F dried over ca	fied, Eastman Kodak er, New York, USA, was everal times from alco- Eastman Kodak Company, alcium chloride and		
were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Meas- urements repeated several times to verify results.		ESTIMATED T/K: prec	ERRORS: cision <u>+</u> 0.1.	r).		

COMPONENTS:

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(1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [120-12-7]
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(2) Benzene; C₆H₆; [71-43-2]

EVALUATOR:

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W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
June, 1994
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CRITICAL EVALUATION:

Biphenyl solubilities in benzene were retrieved from papers by Choi et al. (1), McLaughlin and Zainal (2), Warner et al. (3) and Chang (4). The first three studies report observed values at several temperatures, whereas Chang determined only a single mole fraction solubility for 298 K. There is no a prior reason to exclude any of the four studies from the critical evaluation.

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

 $Ln x_1 = -2233.1 (1/T) + 6.5272 \qquad (r = 0.9998)$ for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.3819$, and differs by less than 1 % from experimental value of $x_1 = 0.381$ (4).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

- Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.
- 2. McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1959, 863-867.
- 3. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. J. Chem. Phys. 1934, 2, 590-594.
- 4. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Methylbenzene; C₇H₈; [108-88- 	-3] Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
±/°C x₂	x 1
25.0 0.62	3 0.377
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a p thermometer.	precision (1) Purity, source and purification proce- dures not specified.
Mixtures of known concentrations in glass ampoules and placed in temperature to equilibrate. Samp were rotated while bath temperatur increased. Solubility determined	sealed (2) Reagent Grade, Eastman Organic Chemical Constant Company, USA, was used as received.
noting the temperature at which trace of solid solute disappeared ubilities at 298 K interpolated experimental values using $\ln x_1 \propto 1/T$ graph.	the last ESTIMATED ERRORS: d. Sol- from T/K : precision \pm 0.1. versus x_1 : \pm 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W. Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
(2) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]				
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂	<i>x</i> ₁			
25.0 0.637	0.363			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.			
noting the temperature at which the last	ESTIMATED ERRORS:			
trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus 1/T graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).			

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] Lee, H.H.; Warner, J.C. (2) Naphthalene; C ₁₀ H ₈ ; [91-20-3] J. Am. Chem. Soc. <u>1935</u> , 57, 318-321. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EIPERIMENTAL VALUES YALANDO 339.3 0.770 334.0 0.700 334.3 0.697 322.8 0.551 318.6 0.500 318.7 0.474 313.0 0.449 313.2 0.448 313.2 0.444 0.555 313.0 312.8 0.444 0.555 313.0		
(1) Biphenyl; $C_{12}H_{10}$; $[92-52-4]$ Lee, H.H.; Warner, J.C.(2) Naphthalene; $C_{10}H_{0}$; $[91-20-3]$ J. Am. Chem. Soc. 1235, 57, 318-321.VARIABLES: TemperaturePREPARED BY: W.E. Acree, Jr. EIPERIMENTAL VALUES Y.K. X2 X1 353.3T/KX2 X2 X1334.00.700334.30.6970.300334.30.6970.303327.50.6070.393326.80.6000.400322.80.5510.449318.60.500315.70.4740.526314.20.4590.550313.00.4470.553312.80.4470.555313.00.4440.555313.00.4440.555313.00.444		
(2) Naphthalene; C ₁₀ H ₈ ; [91-20-3] J. Am. Chem. Soc. <u>1935</u> , 57, 318-321. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EIPERIMENTAL VALUES Y T/K X2 X339.3 0.770 334.0 0.700 334.3 0.697 322.8 0.607 318.6 0.551 318.6 0.500 313.0 0.449 313.0 0.459 313.0 0.450 313.0 0.448 0.550 313.2 313.0 0.447 0.555 313.0 313.0 0.444 0.555 313.0 0.444		
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313.0 0.444 0.556		
315 7 0 427 0 573		
J 313./ U.42/ U.5/3		
316.1 0.400 0.600		
321.0 0.343 0.657		
323.5 0.300 0.700		
331.0 0.194 0.806		
336.7 0.102 0.898		
342.2 0.000 1.000		
AUXILIARY INFORMATION		
METEOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision (1) Highest Purity, Eastman Chemicals recrystallized.	, was	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	, was	
noting the temperature at which the last ESTIMATED ERRORS:		
T/K: precision \pm 0.1. $x_1: \pm 0.001.$	1	

COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.	
(2) 2-Methylnaphthalene; C ₁₁ H ₁₀ ; [91-57-6]		Int. DATA Ser., Ser. A <u>1984</u> , 41.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	*2	x ₁	
307.70	1.0000	0.0000	
304.95	0.9071	0.0929	
302.35	0.8127	0.1873	
301.35	0.7649	0.2351	
301.15	0.7489	0.2511	
300.85	0.7328	0.2672	
300.65	0.7167	0.2833	
300.75	0.6974	0.3026	
300.75	0.6844	0.3156	
300.95	0.6780	0.3220	
301.10	0.6682	0.3318	
301.75	0.6519	0.3481	
302.75	0.6356	0.3644	
304.05	0.6193	0.3807	
311.75	0.5203	0.4797	
319.00	0.4196	0.5804	
325.65	0.3173	0.6827	
331.75	0.2133	0.7867	
337.15	0.1075	0.8925	
342.05	0.0000	1.0000	
<u></u>	· • • • • • • • • • • • • • • • • • • •		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a precision thermometer.		(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.	
in glass ampoules and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly increased. Solubility determined by vigual		(2) Pure Grade, Inst. Chem. Przerobki Wegla, Zabre, Poland, was recrystal- lized thrice from methanol.	
noting the temperature at w trace of solid solute disar	which the last	ESTIMATED ERRORS:	
side of solid solide disappeared.		T/K: precision ± 0.1. $x_1: \pm 0.0005.$	
}			

COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]		Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.	
[581-42-0]		Int. DATA Ser., Ser. A <u>1984</u> , 42.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
т/к	*2	× ₁	
383.35	1.0000	0.0000	
375.65	0.8483	0.1517	
369.45	0.7476	0.2524	
351.75	0.4968	0.5032	
342.95	0.3969	0.6031	
331.65	0.2973	0.7027	
329.55	0.2807	0. 7193	
328.15	0.2724	0.7276	
327.15	0.2641	0.7359	
328.15	0.2476	0.7524	
331.35	0.1979	0.8021	
326.95	0.0988	0.9012	
342.05	0.000	1.0000	
AUXILIARY INFORMATION			
METEOD: APPARATUS/PROCEDURE		SUURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples upper procked while bath temperature class		 Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined. Pure Grade, Schuchardt, Munchen, GFR, was sodium-refined and fractionally crystallized. 	
increased. Solubility det noting the temperature at	ermined by which the last	ESTIMATED ERRORS:	
trace of solid solute disappeared.		T/K: precision ± 0.1. x_1 : ± 0.0005.	

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COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Lee, H.H.; Warner, J.C.	
(2) 1,2-Diphenylethane; C ₁₄ H ₁₄ ; [103-29-7]		J. Am. Chem. Soc. <u>1935</u> , 57, 318-321.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	x 2	x1	
324.5	1.000	0.000	
320.1	0.900	0.100	
316.0	0.800	0.200	
313.3	0.750	0.250	
310.7	0.700	0.300	
308.1	0.650	0.350	
305.6	0.600	0.400	
304.1	0.577	0.423	
305.5	0.567	0.433	
303.1	0.560	0.440	
303.0	0.558	0.442	
302.9	0.557	0.443	
303.0	0.555	0.445	
303.2	0.553	0.447	
303.1	0.550	0.450	
308.0	0.500	0.500	
317.0	0.400	0.600	
324.0	0.300	0.700	
330.7	0.200	0.800	
336.8	0.100	0.900	
342.2	0.000	1.000	
	AUXILIARY	INFORMATION	
AUXILIARY METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a precision thermometer.		(1) Highest Purity, Eastman Chemicals, was recrystallized	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly		(2) Highest Purity, Eastman Chemicals, was recrystallized.	
noting the temperature	at which the last	ESTIMATED ERRORS:	
trace of solid solute disappeared.		T/K: precision ± 0.1. x_1 : ± 0.001.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.	
<pre>(2) 1,2,3,4-Tetrahydronaphthalene; C₁₀H₁₂; [119-64-2]</pre>	Fluid Phase Equilibr. <u>1989</u> , 44, 305-345.	
VARIABLES:	PREPARED BY:	
Temperature	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-+	
т/к x ₂ x ₁	<i>T/K x</i> ₂ <i>x</i> ₁	
305.6 0.5472 0.4528	322.7 0.3292 0.6708	
310.5 0.4940 0.5060	326.9 0.2661 0.7339	
314.6 0.4444 0.5556		
319.2 0.3815 0.6185		
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed	(1) 99.6 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.	
in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.	
noting the temperature at which the last	ESTIMATED ERRORS:	

T/K:	precision	±	0.1.
x1: 1	<u>.</u> 0.0003.		

COMPONENTS:			ORIGINAL	MEASUREMENTS	:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Warner,	J.C.; Scheib	, R.C.; Svirbely, N	W.J.	
(2) 1,4-Dioxane; C ₄ H ₈ O ₂ ; [123-91-1]		J. Chem.	Phys. <u>1934</u>	, 2, 590-594.		
VARIABLES:			PREPARED I	BY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL V	VALUES		· · · · · · · · · · · · · · · · · · ·			
T/K	*2	*1	T/K	<i>x</i> 2	*1	
299.6	0.602	0.398	328.2	0.248	0.752	
305.6	0.543	0.457	330.9	0.204	0.796	
312.5	0.465	0.535	336.6	0.104	0.896	
320.5	0.362	0.638	340.9	0.031	0.969	
326.3	0.275	0.725				
		AUXILIARY	INFORMATION	8		
METHOD: APPARATUS/PROCEDURE		SOURCE ANI	D PURITY OF	MATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Meas-		(1) Purit Compa recry hol.	ty not special any, Rochesto ystallized se	fied, Eastman Koda) er, New York, USA, everal times from a	was alco-	
		was refluxed over metallic sodium and distilled from phosphorous pentoxide.		ind le.		
		ESTIMATED	ERRORS :			
urements repeated several times to verify results.		$T/K: pred x_1: \pm 0.0$	cision \pm 0.1. 02. (compile	er).		

CONDONESTIC		ADIAINAL MENCIDEMENTE.
COMPONENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.
(2) Diphenyl ether; C ₁₂ H ₁₀ O; [101-84-8]		Int. DATA Ser., Ser. A <u>1984</u> , 43.
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
T/K	*2	×1
300.00	1.0000	0.0000
294.35	0.8908	0.1092
289.75	0.7837	0.2163
286.75	0.7310	0.2690
286.05	0.7153	0.2847
289.45	0.6789	0.3211
301.45	0.5761	0.4239
310.95	0.4753	0.5247
318.75	0.3766	0.6234
325.65	0.2797	0.7203
331.95	0.1847	0.8153
337.25	0.0915	0,9085
341.99	0,0000	1,0000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.		(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.
Mixtures of known concent in glass ampoules and pla temperature to equilibrat were rocked while bath te	rations sealed ced in constant e. Samples mperature slowlv	(2) Pure Grade, Fabryka Odczynnikov Chem., Gliwice, Poland, was distilled before use.
increased. Solubility det noting the temperature at	ermined by which the last	ESTIMATED ERRORS:
trace of solid solute disappeared.		$T/K:$ precision \pm 0.1. $x_1: \pm$ 0.0005.
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COMPONENTS	ORIGINAL MEASUREMENTS:
COMPONENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.
(2) Dichloromethane; CH ₂ Cl ₂ ; [75-09-2]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	<i>x</i> ₁
25.0 0.588	0.412
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, J. T. Baker Chemical Company, USA, was used as received.
noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using ln x ₁ versus	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.	
<pre>(2) Trichloromethane; CHCl₃; [67-66-3]</pre>	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/° C x ₂	x 1	
25.0 0.578	0.422	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Eastman Organic Chem- ical, USA, was used as received.	
noting the temperature at which the last trace of solid solute disappeared. Sol-	ESTIMATED ERRORS:	
ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).	

6000000000 00 00 00 00 00 00 00 00 00 00		ADTAINAT MEASIDEMENTS.		
COMPONENTS:		VILVINI MENOVEMENIO:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Acree, W.E., Jr.		
<pre>(2) Tetrachloromethane; CCl₄; [56-23-5]</pre>		Int. J. Pharm. <u>1984</u> , 18, 47-52.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	*2	×1		
25.0	0.6579	0.3421		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIA		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo-		(2) 99.8+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.		
hexane. Concentrations determined spectrophotometrically at 250 nm.		ESTIMATED ERRORS:		
		$T/K: \pm 0.05.$ $x_1: \pm 1 $ (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.		
(2) Tetrachloromethane; CCl ₄ ; [56-23-5]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).		
VARIABLES:	PREPARED BY:		
<i>T/K</i> = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	×1		
25.0 0.658	0.342		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.		
noting the temperature at which the last trace of solid solute disappeared. Sol-	ESTIMATED ERRORS:		
ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).		

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COMPONENTS:			ORIGINAL M	EASUREMENTS	l	
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Tetrachloromethane; CCl₄;</pre>		Warner, J.C.; Scheib, R.C.; Svirbely, W.J. <i>J. Chem. Phys.</i> <u>1934</u> , 2, 590-594.				
VARI	ABLES:			PREPARED E	Y:	
Tem	Temperature		W.E. Acre	W.E. Acree, Jr.		
EXPE	RIMENTAL VA	LUES				_
	T/K	*2	x 1	T/K	*2	×1
	301.3	0.628	0.372	326.8	0.286	0.714
ļ	303.9	0.599	0.401	330.6	0.218	0.782
]	313.2	0.482	0.518	337.5	0.094	0.906
	314.5	0.466	0.534	339.2	0.061	· 0.939
AUXILIARY		INFORMATION	T			
METH	METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF	MATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(1) Purit Compa recry hol. (2) Purit was c disti	y not speci: ny, Rocheste stallized so y not given fried over ca illed shorth	fied, Eastman Kodak er, New York, USA, was everal times from alco- , Eastman Kodak Company, alcium chloride and y before use.	
not tra ure res	increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Meas- urements repeated several times to verify results.		ESTIMATED T/K: prec $x_1: \pm 0.0$	ERRORS: cision <u>+</u> 0.1. 02. (compile		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		McLaughlin, E.; Zainal, H.A.		
<pre>(2) Tetrachloromethane; CCl₄; [56-23-5]</pre>		J. Chem. Soc. <u>1960</u> , 2485-2488.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES	·····			
<i>Т/К х</i> 2		×1		
303.2 0.60	37	0.3963		
311.6 0.50	54	0.4946		
318.6 0.40	02	0.5998		
326.8 0.1721		0.8279		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		 Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant. AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use. 		
		ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003 (compiler).		

COMPONENTS:

 Biphenyl; C₁₂H₁₀; [120-12-7]
 Tetrachloromethane; CCl₄; [56-23-5]

EVALUATOR:

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W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
June, 1994
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CRITICAL EVALUATION:

Biphenyl solubilities in tetrachloromethane were retrieved from papers by McLaughlin and Zainal (1), Warner et al. (2), Acree et al. (3), Acree (4) and Chang (5). The first two studies report observed values at several temperatures, Acree et al. determined values at 303, 308 and 313 K, and Acree and Chang measured only the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the five studies from the critical evaluation.

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

 $Ln x_1 = -2555.1 (1/T) + 7.5025 \qquad (r = 0.9947)$ for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.3438$, and differs by less than 1 % from experimental values of $x_1 = 0.3421$ (4) and $x_1 = 0.342$ (5).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

- 1. McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 2485-2488.
- 2. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. J. Chem. Phys. 1934, 2, 590-594.
- 3. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.
- 4. Acree, W.E., Jr. Int. J. Pharm. 1984, 18, 47-52.
- 5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:	ORIGINAL MEASUREMENTS:				
 Biphenyl; C₁₂H₁₀; [92-52-4] Tetrachloromethane; CCl₄; [56-23-5] 		Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. <u>1986</u> , 31, 225-230.			
VARIABLES:		PREPARED BY	:		
T/K = 303, 308 and 313		W.E. Acree	, Jr.		
EXPERIMENTAL VALUES					
t/°C x ₂	×1	t/°C	*2	×1	
30.0 0.6044	0.3956	40.0	0.4802	0.5198	
35.0 0.5426	0.4574				
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	*	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath, thermometer, and an ultravi spectrophotometer.	(1) 99 %, Milwau lized	Aldrich Cher kee, Wiscons 3 times from	mical Company, sin, USA, recrystal- n methanol.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a		(2) 99.8+ Scient USA, w and di	%, Spectroan ific, Pittsh as stored ov stilled shore	nalyzed, Fisher ourgh, Pennsylvania, ver molecular sieves rtly before use.	
coarse filter into tared volumetric flasks, weighed and diluted with cyclo- hexane. Concentrations determined spectrophotometrically at 250 nm.		ESTIMATED E	RRORS:		

 $T/K: \pm 0.05.$ $x_1: \pm 1$ % (relative error).

COMPONEN 13 :			ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]			Chang, W.		
<pre>(2) 1,2-Dibromoethane; C₂H₄Br₂; [106-93-4]</pre>		; C ₂ H ₄ Br ₂ ;	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).		
VARIABLES:			PREPARED BY:		
<i>T/</i> K = 298			W.E. Acree, Jr.		
EXPERIMENTAL	VALUES				
t	/° C	*2	×1		
25.0 0.611		0.611	0.389		

AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus 1/T graph.	(2) Reagent Grade, Eastman Organic Chem- ical, USA, was used as received.		
	ESTIMATED ERRORS:		
	T/K: precision \pm 0.1. x ₁ : \pm 2 % (relative error; compiler).		

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	ODICINAL MERCIDENENDE		
COMPONENTS:	ORIGINAL MEASUREMENIS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.		
(2) 1,1-Dichloroethane; C ₂ H ₄ Cl ₂ ; [75-34-3]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).		
VARIABLES:	PREPARED BY:		
<i>T/</i> K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES	•		
t/°C x ₂	×1		
25.0 0.619	0.381		
AUXILIARY	INFORMATION		
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.		
noting the temperature at which the last	ESTIMATED ERRORS:		
trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from experimental values using ln x ₁ versus 1/T graph.	T/K: precision \pm 0.1. x ₁ : \pm 2 % (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.		
<pre>(2) 1,2-Dichloroethane; C₂H₄Cl₂; [107-06-2]</pre>	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C ×2	x ₁		
25.0 0.603	0.397		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	 Purity, source and purification proce- dures not specified. 		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.		
noting the temperature at which the last	ESTIMATED ERRORS:		
ubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Chlorobenzene; C ₆ H ₅ Cl; [108-90-7]	Chang, W. Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/° C x ₂	<i>x</i> 1			
25.0 0.603	0.397			
AUXILIARY	INFORMATION .			
METHOD: APPARATUS/PROCEDURE Constant temperature bath and a precision	SOURCE AND PURITY OF MATERIALS: (1) Purity, source and purification proce-			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Sol- ubilities at 298 K interpolated from	<pre>(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received. ESTIMATED ERRORS: T/K: precision + 0.1.</pre>			
experimental values using $\ln x_1$ versus $1/T$ graph.	$x_1: \pm 2$ % (relative error; compiler).			

COMPONENTS:			ORIGINAL MEASUREMENTS:			
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) 1,4-Dichlorobenzene; C₆H₄Cl₂; [106-46-7]</pre>			Warner, J.C.; Scheib, R.C.; Svirbely, W.J. J. Chem. Phys. <u>1934</u> , 2, 590-594.			
Temperature			W.E. Acro	ee, Jr.		
EXPERIMENTAL	VALUES					
T/K	x 2	x 1	T/K	x 2	× 1	
300.9	0.575	0.425	330.6	0.198	0.802	
307.3	0.504	0.496	334.6	0.141	0.859	
314.4	0.425	0.575	338.2	0.077	0.923	
323.0	0.308	0.692				
		AUXILIARY	INFORMATION	N		
METHOD: APPARATUS/PROCEDURE			SOURCE AND	D PURITY OF	MATERIALS:	
Constant temperature bath and a precision thermometer.			(1) Purit Compa recry	ty not speci any, Rochesto ystallized so	fied, Eastman Kodak er, New York, USA, was everal times from alco-	
in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Purity not given, Eastman Kodak Company was used as received.		, Eastman Kodak Company, ived.	
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Meas- urements repeated several times to verify results.			ESTIMATED T/K: prec $x_1: \pm 0.0$	ERRORS: cision <u>+</u> 0.1 002. (compile	er).	

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COMPONENTS:		ORIGINAL MEASUREMENTS:	
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) 1,4-Dichlorobenzene; C₆H₄Cl₂; [106-46-7]</pre>		Morris, R.E.; Cook, W.A.	
		J. Am. Chem. Soc. <u>1935</u> , 57, 2403-2406.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	*2	x ₁	
326.4	1.000	0.000	
322.6	0.931	0.069	
318.2	0.849	0.151	
314.4	0.788	0.212	
308.4	0.690	0.310	
304.0	0.630	0.370	
300.1	0.575	0.425	
302.6	0.540	0.460	
308.2	0.480	0.520	
312.3	0.440	0.560	
317.3	0.379	0.621	
324.0	0.292	0.708	
331.9	0.177	0.823	
336.4	0.106	0.894	
339.5	0.050	0.950	
342.3	0.000	1.000	
· · · · · · · · · · · · · · · · · · ·	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PR	OCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature thermometer.	e bath and a precision	(1) C.P. grade, Eastman Chemicals, was recrystallized from alcohol to give a melting point temperature of 69.1 °C.	
Mixtures of known co in glass ampoules an temperature to equi were rotated while h	oncentrations sealed nd placed in constant librate. Samples bath temperature slowly	 (2) Purity and chemical source were not specified, was purified by distilla- tion. 	
increased. Solubilit noting the temperate	ty determined by ure at which the last	ESTIMATED ERRORS:	
trace of solid solut	te disappeared.	$T/K:$ precision \pm 0.1. $x_1: \pm$ 0.001.	

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COMPONENTS:			ORIGINAL M	EASUREMENTS :		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]			McLaughli	n, E.; Messe	r, C.E.	
(2) Hexafluor	(2) Hexafluorobenzene; C ₆ F ₆ ; [392-56-3]			J. Chem. Soc., Sect. A <u>1966</u> , 1106-1110.		
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acre	e, Jr.			
EXPERIMENTAL V	ALUES					
T/K	x 2	×1	T/K	×2	x 1	
307.45	0.5954	0.4046	331.35	0.2097	0.7903	
310.95	0.5528	0.4472	331.75	0.2025	0.7975	
314.85	0.5031	0.4969	336.55	0.1077	0.8923	
321.30	0.3992	0.6008	337.30	0.0934	0.9066	
326.70	0.3018	0.6982			•	
		AUXILIARY	INFORMATION	1		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly		(1) Purit Teerv colum	y not given, erwertung, p n, recrystal	Gesellschaft fur assed over alumina lized and sublimed.		
		(2) Purit Ltd, anhyd	y not given, Avonmouth, B rous calcium	Imperial Smelting, ristol, was dried over sulfate.		
noting the te	increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED	ERRORS:		
trace of 8011			$\frac{T/K: \text{ prec}}{x_1: \pm 0.0}$	ision <u>+</u> 0.1. 003.		

COMPONENTS .	ORTGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. <u>1985</u> , 19, 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	· · · · · · · · · · · · · · · · · · ·
±/°C	(mol dm ⁻³)
25.0 0.69	913
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection. Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped	 Highest available commercial purity, specific chemical supplier not given, was used as received. 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
with flame ionization detector and on 10 % SE30 ultraphase column.	ESTIMATED ERRORS: $T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (relative error; compiler).

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COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Berchiesi, G.	
(2) 1-Octadecanol; C ₁₈ H ₃₈ O; [112-92-5]		Int. DATA Ser., Ser. A <u>1985</u> , 95.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EIPERIMENTAL VALUES			
T/K	*2	x 1	
331.2	1.0000	0.0000	
330.3	0.9793	0.0207	
329.3	0.9366	0.0634	
328.2	0.8786	0.1214	
327.6	0.8013	0.1987	
325.9	0.7006	0.2994	
324.4	0.5880	0.4120	
325.0	0.5019	0.4981	
329.8	0.3892	0.6108	
332.3	0.3192	0.6808	
334.3	0.2477	0.7523	
336.4	0.1649	0.8351	
338.6	0.0967	0.9033	
340.8	0.0344	0.9656	
342.3	0.0000	1.0000	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a thermometer.	precision	(1) 98 %, C. Erba, Milano, Italy, was used as received.	
Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly		(2) 99 %, Analytical Reagent, Fluka, St. Gallen, Switzerland, was used as re- ceived.	
noting the temperature at which	the first	ESTIMATED ERRORS:	
trace or solid solute appeared.		$T/K:$ precision \pm 0.1. $x_1: \pm$ 0.001.	
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COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Lee, H.H.; Warner, J.C.	
(2) Benzophenone; C ₁₃ H ₁₀ O; [119-61-9]		J. Am. Chem. Soc. <u>1933</u> , 55, 209-214.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K ×	2	x 1	
326.0 1	.000	0.000	
308.2 0	.772	0.228	
303.5 0	.693	0.307	
299.1 0	.628	0.372	
298.4 0	.607	0.393	
301.2 0	. 575	0.425	
305.5 0	.530	0.470	
311.7 0	.458	0.542	
319.3 0	.362	0.638	
329.4 0	.220	0.780	
342.2 0	.000	1.000	
	AUXILIARY	INFORMATION	
Constant temperature bath and thermometer.	a precision	 (1) Highest Purity, Eastman Chemicals, was recrystallized from alcohol. 	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		 (2) Highest Purity, Eastman Chemicals, was distilled under reduced pressure. ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 0.001. 	

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Chang, W.		
(2) Carbon disulfide; CS ₂ ; [75-15-0]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	×1		
25.0 0.631	0.369		
AUXILI	RY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	 (1) Purity, source and purification proce- dures not specified. 		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slow increased. Solubility determined by	(2) Reagent Grade or better, source not specified, was used as received.		
noting the temperature at which the last trace of solid solute disappeared. Sol-	ESTIMATED ERRORS:		
ublities at 298 K interpolated from experimental values using ln x, versus 1/T graph.	T/K: precision \pm 0.1. x ₁ : \pm 2 % (relative error; compiler).		

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COMPONENTS :		ORIGINAL N	EASUREMENTS	1	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Warner, S	J.C.; Scheib	, R.C.; Svirbely, W.J.	
(2) Carbon di	sulfide; CS ₂	; [75-15-0]	J. Chem. Phys. <u>1934</u> , 2, 590-594.		
VARIABLES:		PREPARED I	BY:		
Temperature		W.E. Acre	ee, Jr.		
EXPERIMENTAL V	ALUES				
T/K	*2	×1	T/K	*2	×1
301.6	0.596	0.404	317.3	0.405	0.595
309.8	0.502	0.498	320.8	0.363	0.637
310.9	0.486	0.514	322.7	0.326	0.674
311.4	0.480	0.520	324.5	0.306	0.694
313.9	0.447	0.553	331.5	0.190	0.810
		AUXILIARY	INFORMATION	4	
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	D PURITY OF N	MATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(1) Purit Compa recry hol. (2) Purit	ty not specif any, Rocheste ystallized se ty not given,	fied, Eastman Kodak er, New York, USA, was everal times from alco- , Eastman Kodak Company,	
		was dried over calcium chloride and distilled twice from mercury.		alcium chloride and from mercury.	
noting the te trace of soli	mperature at d solute dia	which the last	ESTIMATED	ERRORS :	
urements reperents reperents.	ated several	times to verify	T/K: pred x ₁ : ± 0.0	cision <u>+</u> 0.1. 02. (compile	er).

COMPONENTS:		ORIGINAL M	EASUREMENTS :		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Choi, P.E	.; McLaughli	n, E.	
(2) Pyridine;	C ₅ H ₅ N; [110-	86-1]	Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-51.		
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES	· · · · · · · · · · · · · · · · · · ·			
T/K	*2	x 1	T/K	*2	*1
297.3	0.6258	0.3742	323.7	0.3116	0.6884
300.9	0.5915	0.4085	331.7	0.1830	0.8170
307.1	0.5257	0.4743			
312.4	0.4673	0.5327			•
		AUXILIARY	INFORMATION	r	
METHOD: APPARA	METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.		(1) 99 %, Milwa as re	Aldrich Che uukee, Wiscon ceived.	mical Company, sin, USA, was used	
in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.		<pre>%, Aldrich Chemical as received.</pre>	
noting the te	emperature at	which the last	ESTIMATED	ERRORS :	
	a solute dis	abheared.	T/K: prec x ₁ : ± 0.0	cision <u>+</u> 0.1. 003.	

COMPONENTS :		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Choi, P.E	3.; McLaughli	n, E.	
(2) Thiophene; C ₄ H ₄ S; [110-02-1]		Ind. Eng.	Chem. Funda	m. <u>1983</u> , 22, 46-51.	
VARIABLES:			PREPARED B	3Y:	
Temperature		W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES				
T/K	*2	x 1	T/K	*2	×1
295.9	0.6149	0.3851	329.5	0.2347	0.7653
298.4	0.5929	0.4071	334.8	0.1302	0.8698
309.7	0.4782	0.5218			
317.0	0.3940	0.6060			
		AUXILIARY	INFORMATION	r	
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.		(1) 99 %, Milwa as re	Aldrich Che ukee, Wiscon ceived.	mical Company, sin, USA, was used	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.		<pre>%, Aldrich Chemical as received.</pre>	
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED T/K: prec x ₁ : ± 0.0	ERRORS: :ision <u>+</u> 0.1. 003.		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]		Yokoyama, C.; Ebina, T.; Takahashi, S.		
(2) Indole; C ₈ H ₇ N; [120-72-9]		J. Chem. Eng. Data <u>1993</u> , 38, 583-586.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	<i>x</i> ₂	* 1		
326.26	1.0000	0.0000		
317.55	0.8978	0.1022		
310.08	0.8002	0.1998		
306.45	0.7530	0.2470		
301.76	0.6995	0.3005		
301.45	0.6826	0.3174		
304.01	0.6538	0.3462		
308.08	0.6098	0.3902		
312.57	0.5565	0.4435		
318.19	0.4637	0.5363		
323.66	0.3709	0.6291		
328.51	0.2864	0.7136		
335.36	0.1436	0.8564		
343.13	0.0000	1.0000		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath a thermometer.	nd a precision	(1) 99.8 %, Wako Pure Chemical Ind Ltd., was used as received.		
Mixtures of known concentra in glass ampoules and place temperature to equilibrate. were rotated while bath tem increased. Solubility deter	tions sealed d in constant Samples perature slowly mined by	(2) 99.9 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.		
noting the temperature at w	hich the last	ESTIMATED ERRORS:		
Line of solid solute disap	heared.	T/K: precision \pm 0.02. x_1 : \pm 0.0001.		
<u>}</u>				

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.
(2) Indole, Cana, [120-72-5]	Int. DATA Ser., Ser. A <u>1984</u> , 46.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
<i>т/к x</i> 2	×1
324.95 1.0000	0.0000
318.75 0.9222	0.0778
312.65 0.8404	0.1596
306.45 0.7544	0.2456
302.05 0.6945	0.3055
302.70 0.6638	0.3362
310.95 0.5683	0.4317
317.65 0.4674	0.5326
323.85 0.3607	0.6393
329.75 0.2476	0.7524
333.90 0.1644	0.8356
335.75 0.1276	0.8724
337.00 0.1027	0.8973
341.99 0.0000	1.0000
AUXIL	JARY INFORMATION
Constant temperature bath and a precisi- thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constan temperature to equilibrate. Samples were rocked while bath temperature slow increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.	 on (1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined. (2) Pure Grade, Inst. Chem. Przerobki Wegla, Zabre, Poland, was recrystal- lized thrice from methanol. t ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 0.0005.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
 (1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Diphenylamine; C₁₂H₁₁N; [122-39-4] 		Lee, H.H.; Warner, J.C.		
		J. Am. Chem. Soc. <u>1933</u> , 55, 209-214.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	*2	x 1		
326.0	1.000	0.000		
317.7	0.820	0.180		
309.2	0.695	0.305		
306.8	0.646	0.354		
303.5	0.603	0.397		
302.8	0.587	0.417		
304.0	0.565	0.435		
307.3	0.533	0.467		
308.2	0.422	0.478		
312.2	0.477	0.523		
316.9	0.425	0.575		
321.8	0.354	0.646		
326.9	0.268	0.732		
334.1	0.155	0.845		
342.2	0.000	1.000		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath a thermometer.	nd a precision	 Highest Purity, Eastman Chemicals, was recrystallized from alcohol. 		
Mixtures of known concentratin glass ampoules and place temperature to equilibrate. were rotated while bath tem increased. Solubility data	ations sealed ed in constant Samples operature slowly mined by	(2) Highest Purity, Eastman Chemicals, was distilled under reduced pressure.		
noting the temperature at w	which the last	ESTIMATED ERRORS:		
trace of solid solute disar	peareu.	T/K: precision ± 0.1. x_1 : ± 0.001.		
		I		

n	n	n
2	υ	υ

COMPONENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]		ORIGINAL MEASUREMENTS:			
		Srivastava, R.D.; Gupta, P.D. J. Indian Chem. Soc. <u>1967</u> , 44, 960-963.			
					VARIABLES:
Temperature			W.E. Acr	ee, Jr.	
EXPERIMENTAL V	VALUES		I		
T/K	×2	<i>x</i> ₁	T/K	x2	<i>*</i> 1
281.4	0.7858	0.2142	302.2	0.6056	0.3944
291.4	0.6988	0.3012	305.0	0.5808	0.4192
296.0	0.6586	0.3414	311.2	0.5093	0.4907
298.4	0.6399	0.3601			
		AUXILIARY	INFORMATIO	N	
METHOD: APPARI	ATUS/PROCEDUR	E	SOURCE ANI	D PURITY OF M	ATERIALS:
Constant temp thermometer.	perature bath	and a precision	(l) Purit Unite subli	ty not given, ed Kingdom, w Lmed.	British Drug Houses, as recrystallized and
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(2) Purit was c	ty not given, lried and dis	British Drug Houses, tilled.	
		ESTIMATED T/K: prec x ₁ : ± 3 %	ERRORS: cision <u>+</u> 0.1. (relative en	rror, Compiler).	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Ristonia C W (02 52 4)		Berchiegi G
<pre>(1) Bipheny1; C₁₂H₁₀; [92-52-4] (2) 1-Octadecanoic acid; C₁₈H₃₆O₂; [57-11-4]</pre>		Tat DATA for for a 1985 96
		INT. DATA SET., SET. A <u>1985</u> , 96.
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		<u> </u>
T/K	*2	x ₁
339.3	1.0000	0.0000
338.7	0.9726	0.0274
338.0	0.9333	0.0667
335.5	0.7873	0.2127
334.4	0.7249	0.2751
332.4	0.6373	0.3627
330.7	0.5570	0.4430
329.9	0.5100	0.4900
328.3	0.4478	0.5522
327.7	0.4106	0.5894
329.3	0.3783	0.6217
331.0	0.3425	0.6575
332.8	0.3019	0.6981
334.6	0.2544	0.7456
336.4	0.2000	0.8000
337.7	0.1553	0.8447
339.2	0.1054	0.8946
341.3	0.0371	0.9629
342.3	0.0000	1.0000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.		(1) 98 %, C. Erba, Milano, Italy, was used as received.
Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual		(2) 99 %, Schuchardt, Hohenbrunn, Germany, was used as received.
noting the temperature at which	ch the first	ESTIMATED ERRORS:
trace of solid solute appeared.		T/K: precision ± 0.1. x_1 : ± 0.001.

2,2'-BIPYRIDINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

- A. Saturated Hydrocarbons (including cycloalkanes)
- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons
- D. <u>Esters</u>
- E. <u>Ethers</u>
- F. Haloalkanes and Haloaromatic Hydrocarbons

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- G. Alcohols
- H. Ketones
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

methanol + water ethanol + water 2-methyl-2-propanol + water

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2 -Bipyridine; C ₁₀ H ₈ N ₂ ; [366-18-7]	Burgess, J.; Haines, R.I.
(2) Methanol; CH ₄ O; [67-56-1]	Chem. Ind. (London) <u>1980</u> , 289.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a $t = 25.0 ^{\circ}C$	
¢2 ^(s)	c ₁ /(mol dm ⁻³)
0.00	0.037
0.10	0.063
0.20	0.116
0.30	0.240
0.40	0.60
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, and an ultra- violet/visible spectrophotometer. Excess solute and binary solvent equili- brated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectro- metrically at 283 nm. Attainment of equilibrium verified by several repeti- tive measurements.	 Purity and chemical source not specified, was recrystallized from aqueous- ethanol. Purity and chemical source not specified in paper. Purity and chemical source not specified in paper.
	ESTIMATED ERRORS: $T/K: \pm 0.1$ (Compiler). $\phi_2^{(S)}: \pm 0.01$ (Compiler). $c_1: \pm 3$ % (relative error, Compiler).

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COMPONENTS:
                                                                   ORIGINAL MEASUREMENTS:
 (1) 2,2'-Bipyridine; C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>; [366-18-7]
                                                                     Burgess, J.; Haines, R.I.
 (2) Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5]
                                                                     Chem. Ind. (London) 1980, 289.
 (3) Water; H<sub>2</sub>O; [7732-18-5]
VARIABLES:
                                                                   PREPARED BY:
 T/K = 298, Solvent composition
                                                                     W.E. Acree, Jr.
EXPERIMENTAL VALUES<sup>a</sup>
t = 25.0 °C
                         φ2<sup>(s)</sup>
                                                                             c_1/(mol dm^{-3})
                                                                             0.037
                         0.00
                         0.10
                                                                             0.114
                        0.20
                                                                             0.240
                         0.30
                                                                             0.76
      ^a \phi_2^{(s)}; initial volume fraction of binary solvent mixture; c_1; solubility of the solute expressed in terms of molarity.
                                                   AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE
                                                                   SOURCE AND PURITY OF MATERIALS:

    Purity and chemical source not speci-
fied, was recrystallized from aqueous-
ethanol.

 Constant temperature bath, and an ultra-
 violet/visible spectrophotometer.
Excess solute and binary solvent equili-
brated in a constant temperature vessel.
Aliquots of saturated solution withdrawn
                                                                     (2) Purity and chemical source not speci-
                                                                           fied in paper.
 and concentrations determined spectro-
                                                                     (3) Purity and chemical source not speci-
fied in paper.
 metrically at 283 nm. Attainment of
 equilibrium verified by several repeti-
 tive measurements.
                                                                   ESTIMATED ERRORS:
                                                                     \begin{array}{l} T/K: \pm 0.1 \ (Compiler). \\ \phi_2^{(s)}: \pm 0.01 \ (Compiler). \\ c_1: \pm 3 \ \ (relative \ error, \ Compiler). \end{array}
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OMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2,2 [°] -Bipyridine; C ₁₀ H ₂ N ₂ ; [366-18-7]	Burgess, J.; Haines, R.I.	
(2) 2-Methyl-2-propanol; C ₄ H ₁₀ O;	Chem. Ind. (London) <u>1980</u> , 289.	
[75-65-0] (3) Water; H ₂ O; [7732-18-5]		
ARIABLES:	PREPARED BY:	
T/K = 298, Solvent composition	W.E. Acree, Jr.	
IPERIMENTAL VALUES^a t = 25.0 °C	+	
φ ₂ (s)	c ₁ /(mol dm ⁻³)	
0.00	0.037	
0.05	0.078	
0.10	0.120	
0.15	0.195	
0.20	0.33	
0.25	0.92	
^a φ ₂ ⁽³⁾ : initial volume fraction of bina of the solute expressed in terms of mo	ry solvent mixture; c ₁ : solubility larity.	
^a φ ₂ ⁽³⁾ : initial volume fraction of bina of the solute expressed in terms of mo	ry solvent mixture; c ₁ : solubility larity.	
^a φ ₂ ⁽³⁾ : initial volume fraction of bina of the solute expressed in terms of mo AUXILIAR	Y INFORMATION	
^a φ ₂ ⁽³⁾ : initial volume fraction of bina of the solute expressed in terms of mo AUXILIAR ETEOD: APPARATUS/PROCEDURE	Y INFORMATION SOURCE AND FURITY OF MATERIALS:	
Φ ₂ ^(S) : initial volume fraction of bina of the solute expressed in terms of mo AUXILIAR ETHOD: APPARATUS/PROCEDURE Constant temperature bath, and an ultra- violet/visible spectrophotometer.	Y INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source not speci- fied, was recrystallized from aqueous- ethanol.	
AUXILIAR ETEOD: APPARATUS/PROCEDURE Constant temperature bath, and an ultra-violet/visible spectrophotometer. Excess solute and binary solvent equiliprated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectro-	Y INFORMATION SOURCE AND FURITY OF MATERIALS: (1) Purity and chemical source not speci- fied, was recrystallized from aqueous- ethanol. (2) Purity and chemical source not speci- fied in paper.	
AUXILIAR AUXILIAR ETHOD: APPARATUS/PROCEDURE Constant temperature bath, and an ultraviolet/visible spectrophotometer. Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of aquilibrium verified by several repetitive measurements.	Y INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source not speci- fied, was recrystallized from aqueous- ethanol. (2) Purity and chemical source not speci- fied in paper. (3) Purity and chemical source not speci- fied in paper.	
AUXILIAR AUXILIAR ETHOD: APPARATUS/PROCEDURE Constant temperature bath, and an ultra-violet/visible spectrophotometer. Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectro-metrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.	Y INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source not speci- fied, was recrystallized from aqueous- ethanol. (2) Purity and chemical source not speci- fied in paper. (3) Purity and chemical source not speci- fied in paper.	
AUXILIAR AUXILIAR ETHOD: APPARATUS/PROCEDURE Constant temperature bath, and an ultraviolet/visible spectrophotometer. Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.	Y INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source not speci- fied, was recrystallized from aqueous- ethanol. (2) Purity and chemical source not speci- fied in paper. (3) Purity and chemical source not speci- fied in paper.	

BUCKMINSTERFULLERENE	SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES
А.	Saturated Hydrocarbons (including cycloalkanes)
	n-pentane
	n-hexane
	n-octane
	n-decane
	n-dodecane
в.	Alkenes
с.	Aromatic Hydrocarbons
	benzene ·
	methylbenzene
	ethylbenzene
	n-propylbenzene
	iso-propylbenzene
	n-butylbenzene
	sec-butylbenzene
	t-butylbenzene
	1,2-dimethylbenzene
	1,3-dimethylbenzene
	1,4-dimethylbenzene
	1,2,3-trimethylbenzene
	1,2,4-trimethylbenzene
	1,3,5-trimethy1benzene
	1,2,3,4-tetramethylbenzene
	1,2,3,5-tetramethylbenzene
	1,2,3,4-tetrahydronaphthalene
	1-methylnaphthalene
D.	Esters
E.	Ethers
	1,4-dioxane
	methoxybenzene
F.	Haloalkanes_and_Haloaromatic_Hydrocarbons
	dichloromethane
	trichloromethane
	tetrachloromethane
	1,2-dibromoethane
	tetrachloroethylene
	1,1,2,2-tetrachloroethane
	bromobenzene
	chlorobenzene
	1,2-dibromobenzene
	1,3-dibromobenzene
	1,2-dichlorobenzene
	1,3-dichlorobenzene
	1,2,4-trichlorobenzene
	fluorobenzene
iodobenzene 1-bromo-2-methylnaphthalene

G. Alcohols

2-hydroxymethylbenzene

- H. <u>Ketones</u>
- I. <u>Miscellaneous</u> Pure_Solvents

carbon disulfide benzonitrile nitrobenzene pyridine quinoline thiophene 2-methylthiophene tetrahydrothiophene

J. Binary Solvent Mixtures

	-
COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n-Pentane; C₅H₁₂; [109-66-0]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
<i>T</i> /K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	-
t/°C c ₁ /	(mol dm ⁻³)
30.0 5.5	5 × 10 ⁻⁶
AUTT.TARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS:
	T/K: \pm 0.1. c ₁ : \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; [99685-96-8] (2) n-Pentane; C ₅ H ₁₂ ; [109-66-0]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 8 x	10-7
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

CONDONENTICS	OPTOINST MESSIPENENTS.
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n-Hexane; C₆H₁₄; [110-54-3]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
30.0 5.55×10^{-5}	
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS:
	T/K: \pm 0.1. c_1 : \pm 3 % (relative error; compiler).

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n-Hexane; C₆H₁₄; [110-54-3]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 7.3	x 10 ⁻⁶
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96~8] (2) n-Octane; C₈H₁₈; [111-65-9]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
30.0 3.4	7 x 10 ⁻⁵
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS: T/K: ± 0.1. c ₁ : ± 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n-Decane; C₁₀H₂₂; [124-18-5]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
30.0 9.7	1 x 10 ⁻⁵
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS:
	$T/K: \pm 0.1.$ c ₁ : ± 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n=Decane; C:Ha; (124-18-5)</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2)	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 1.9	x 10 ⁻⁵
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n-Dodecane; C₁₂H₂₆; [112-40-3]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
<i>T/K</i> = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
30.0 1.2	6 x 10 ⁻⁴
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS:

T/K: \pm 0.1. c₁: \pm 3 % (relative error; compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Buckminsterfullerene; C₆₀; Sivaraman, N.; Dhamodaran, R.; Kaliappan, [99685-96-8] I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. (2) Benzene; C₆H₆; [71-43-2] 1992, 57, 6077-6079. PREPARED BY: VARIABLES: T/K = 303W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(mol dm^{-3})$ t/°C 2.00×10^{-3} 30.0 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with-and the absorbance measured at 328 nm after appropriate dilution with spectro-scopic grade n-bewane. sample purified by chromatographic separation on alumina column. (2) HPLC grade or AR grade solvent, chem-ical source not given, aromatic impuri-ties removed by chromatography if necessary. scopic grade n-hexane. ESTIMATED ERRORS: T/K: \pm 0.1. c₁: \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; [99685-96-8] (2) Benzene; C ₆ H ₆ ; [71-43-2]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , <i>97</i> , 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C x ₁	
22 2.1	x 10 ⁻⁴
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Scrivens, W.A.; Tour, J.M.
(2) Benzene; C ₆ H ₆ ; [71-43-2]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /(mol dm ⁻³)
22 2.1	x 10 ⁻³
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
restaue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.

COMPONENTS: (1) Buckminsterfullerene; C ₆₀ ; [99685-96-8] (2) Mothylbonzone; C.W.; [108-88-3]	ORIGINAL MEASUREMENTS: Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Vathour, C.K.
	J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
<i>T</i> /K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	mol dm ⁻³)
30.0 2.98	3 × 10 ⁻³
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
<u> </u>	ESTIMATED ERRORS: $T/K: \pm 0.1.$ $c_1: \pm 3$ % (relative error; compiler).

ORIGINAL MEASUREMENTS:
Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
PREPARED BY:
W.E. Acree, Jr.
0×10^{-4}
INFORMATION
SOURCE AND PURITY OF MATERIALS:
 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
ESTIMATED ERRORS: $T/K: \pm 3.$ $x_i: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) Metnyibenzene; C ₇ n ₈ ; [100-00-3]	1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	$c_1/(mol dm^{-3})$
22	4.0×10^{-3}

ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid residue.	 Purity and chemical source were not given in the paper. Purity and chemical source were not given in the paper.
	ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
[99685-96-8] (2) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C c ₁ /	(mol dm ⁻³)	
22 3.6	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler), $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) n-Propylbenzene; C₉H₁₂; [103-65-1]</pre>	Scrivens, W.A.; Tour, J.M. <i>J. Chem. Soc., Chem. Commun.</i> <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
±/°C c ₁ //	(mol dm ⁻³)	
22 2.1	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	 (1) Purity and chemical source were not given in the paper. (2) Purity and chemical source were not given in the paper. 	
residue.	ESTIMATED ERRORS:	

STIMATED ERRORS:

 $T/K: \pm 3$ (Compiler), c₁: ± 0.0007 mol dm⁻³.

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
(2) iso-Propylbenzene; C ₉ H ₁₂ ; [98-82-8]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C c ₁ /(c ₁ /(mol dm ⁻³)	
22 1.7	x 10 ⁻³	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). c ₁ : ± 0.0007 mol dm ⁻³ .	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Scrivens, W.A.; Tour, J.M.	
(2) n-Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C C ₁ /((mol dm ⁻³)	
22 2.6	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge. Excess solute and solvent allowed to	 Purity and chemical source were not given in the paper. 	
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). c ₁ : ± 0.0007 mol dm ⁻³ .	

-	1	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) sec-Butylbenzene; C₁₀H₁₄; [135-98-8]</pre>	Scrivens, W.A.; Tour, J.M. <i>J. Chem. Soc., Chem. Commun.</i> <u>1993</u> , 1207- 1209.	
	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_1/(mol dm^{-3})$		
22 1.5	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	 (1) Purity and chemical source were not given in the paper. (2) Purity and chemical source were not given in the paper. 	
residue.	ESTIMATED ERRORS: $T/K: \pm 3$ (Compiler), $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ; (99685-96-8)	Scrivens, W.A.; Tour, J.M.	
(2) t-Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C c ₁ /	mol dm ⁻³)	
22 1 x	10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
equilibrate in a room temperature bath	(2) Purity and chemical source were not	
for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a	given in the paper.	
0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared		
vials, which were then placed in a heated oil bath to facilitate solvent evapora-		
tion. Concentrations determined gravi-		
residue.		
	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler), c ₁ : ± 0.0007 mol dm ⁻³ .	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,2-Dimethylbenzene; C₈H₁₀;</pre>	Scrivens, W.A.; Tour, J.M. J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207-	
[95-47-6]	1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_1/(mol dm^{-3})$		
22 1.2	x 10 ⁻²	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

60100100000		
COMPONENTS	UKIGINAL MEASUKEMENIS:	
<pre>(1) Buckminsterfullerene; C₆₀; (99685-96-8)</pre>	Scrivens, W.A.; Tour, J.M.	
(2) 1,3-Dimethylbenzene; C ₈ H ₁₀ ; [108-38-3]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /	(mol dm ⁻³)	
22 1.9	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). c ₁ : $\pm 0.0007 \text{ mol dm}^3$.	

	7	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,4-Dimethylbenzene; C₈H₁₀; [106-42-3]</pre>	Scrivens, W.A.; Tour, J.M. <i>J. Chem. Soc., Chem. Commun.</i> <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
<pre>T/K = Circa 295 (Ambient Room)</pre>	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
$t/^{\circ}C$ $c_{1}/(mol dm^{-3})$		
22 8.2	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler),	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
<pre>(2) 1,2,3-Trimethylbenzene; C₉H₁₂; [526-73-8]</pre>	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
±/°C c ₁ /(mol dm ⁻³)	
22 6.5	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
,	$T/K: \pm 3$ (Compiler), $c_1: \pm 0.0007 \text{ mol dm}^3$.	

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; (99685-96-8)</pre>	Scrivens, W.A.; Tour, J.M.
(2) 1,2,4-Trimethylbenzene; C ₉ H ₁₂ ; [95-63-6]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
22 2.4	18 x 10 ⁻²
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler). c ₁ : \pm 0.0007 mol dm ⁻³ .

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,3,5-Trimethylbenzene; C₉H₁₂; [108-67-8]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 303	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	c ₁ /(mol dm ⁻³)	
30.0	1.38 × 10 ⁻³	
AUXILIARY INFORMATION		

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro-	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS: $T/K: \pm 0.1.$ $c_1: \pm 3$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,3,5-Trimethylbenzene; C₉H₁₂; [108-67-8]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 3.1	x 10 ⁻⁴
AUXILIARY	INFORMATION
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,3,5-Trimethylbenzene; C₉H₁₂; [108-67-8]</pre>	Scrivens, W.A.; Tour, J.M. J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /(mol dm ⁻³)	
22 2.4	x 10 ⁻³	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$c_1: \pm 0.0007 \text{ mol } dm^{-3}.$	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Scrivens, W.A.; Tour, J.M.
(2) 1,2,3,4-Tetrametnyibenzene; C ₁₀ H ₁₄ ; [488-23-3]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
22 8.0	x 10 ⁻²
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a	(2) Purity and chemical source were not given in the paper.
0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated	
oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	
residue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler). c ₁ : \pm 0.0007 mol dm ⁻³ .

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,2,3,5-Tetramethylbenzene; C₁₀H₁₄; [527-53-7]</pre>	Scrivens, W.A.; Tour, J.M. <i>J. Chem. Soc., Chem. Commun.</i> <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C c ₁ /	(mol dm ⁻³)	
22 2.8	9 x 10 ⁻²	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid residue.	 (1) Purity and chemical source were not given in the paper. (2) Purity and chemical source were not given in the paper. ESTIMATED ERRORS: T/K: ± 3 (Compiler), 	
	T/K: ± 3 (Compiler). c ₁ : ± 0.0007 mol dm ⁻³ .	

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Buckminsterfullerene; C₆₀; [99685-96-8] 1,2,3,4-Tetrahydronaphthalene; C₁₀H₁₂; [119-64-2] 	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C ×1	
22 3.1	x 10 ⁻⁵
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.	
[2] 1-Methylnaphthalene; C ₁₁ H ₁₀ ; [90-12-0]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₁		
22 6.8	x 10 ⁻⁵	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec-	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer. 	
tion at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:	

 x_1 : \pm 8 % (relative error; compiler).

and the second		
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
(2) 1-Methylnaphthalene; C ₁₁ H ₁₀ ; [90-12-0]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /(mol dm ⁻³)	
22 4.6	L x 10 ⁻²	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler), $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,4-Dioxane; C₄H₈O₂; [123-91-1]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. <i>J. Org. Chem.</i> <u>1992</u> , 57, 6077-6079.	
VARIABLES:	PREPARED BY:	
T/K = 303	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /((mol dm ⁻³)	
30.0 5.6	9 x 10 ⁻⁵	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary. 	
	ESTIMATED ERRORS: $T/K: \pm 0.1.$ $c_1: \pm 3$ % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Buckminsterfullerene; C₆₀; [99685-96-8] Methoxybenzene; C₇H₈O; [100-66-3] 	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , <i>9</i> 7, 3379-3383.
VARIABLES:	PREPARED BI:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 8.4	x 10 ⁻⁴
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$
	$ x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Dichloromethane; CH₂Cl₂; [75-09-2]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. <i>J. Org. Chem.</i> <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /(mol dm ⁻³)
30.0 3.5	2 x 10 ⁻⁴
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary.
	ESTIMATED ERRORS:
	$T/K: \pm 0.1.$ $c_1: \pm 3$ % (relative error; compiler).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; [99685-96-8]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) Dichloromethane; CH ₂ Cl ₂ ; [75-09-2]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 2.7	x 10 ⁻⁵
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; [99685-96-8]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) IFICHIOFOMECHANE; CHCI ₃ ; [67-66-5]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C x ₁	
22 2.2	x 10 ⁻⁵
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer. Reported to con- tain 1 % ethanol as a stabilizer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Sivaraman, N.; Dhamodaran, R.; Kaliappan,	
[99685-96-8]	I., Srinivasan, R.G.; Vasudeva Rao, P.R.;	
(2) Tetrachloromethane; CCl ₄ ; [56-23-5]	Mathews, C.K.	
	J. Org. Chem. <u>1992</u> , 57, 6077-6079.	
VARIABLES:	PREPARED BY:	
T/K = 303	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°c c ₁ /	(mol dm ⁻³)	
30.0 6.2	6.20×10^{-4}	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary. 	
	ESTIMATED ERRORS:	
	T/K: \pm 0.1. c ₁ : \pm 3 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Tetrachloromethane; CCl₄; [56-23-5] 	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 4.0	x 10 ⁻⁵
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
 High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a 	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(106-93-4)	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 6.0	x 10 ⁻⁵
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ X: + 8 % (relative error: compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Tetrachloroethylene; C₂Cl₄; [127-18-4] 	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , <i>97</i> , 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 1.7	x 10 ⁻⁵
AUXILIARY	INFORMATION
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: T/K: ± 3.
	$x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,1,2,2-Tetrachloroethane; C₂H₂Cl₄; [79-34-5]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 7.7	x 10 ⁻⁴
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Bromobenzene; C₆H₅Br; [108-86-1]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 4.8	x 10 ⁻⁴
AUXILIARY	INFORMATION
AUXILIARY	INFORMATION Source and purity of materials:
AUXILIARY METHOD: APPARATUS/PROCEDURE High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.</pre>

phase was used.

T/K: \pm 3. x₁: \pm 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; (99685-96-8)</pre>	Scrivens, W.A.; Tour, J.M.
(2) Bromobenzene; C ₆ H ₅ Br; [108-86-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
22 3.9	x 10 ⁻³
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath	(2) Purity and chemical source were not
for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a	given in the paper.
0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared	
vials, which were then placed in a heated oil bath to facilitate solvent evapora-	
tion. Concentrations determined gravi- metrically from the weight of the solid	
residue.	ESTIMATED EPROPS:
	$c_1: \pm 0.0007 \text{ mol } dm^{-3}$.

COMPONENTS: (1) Buckminsterfullerene; C ₆₀ ; [99685-96-8]	ORIGINAL MEASUREMENTS: Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) Chlorobenzene; C ₆ H ₅ Cl; [108-90-7]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 9.9	x 10 ⁻⁴
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina
Excess solute and solvent placed in 1-dram glass bottle and allowed to equili-	column. Final purity of 99.95 % as determined by mass spectrometry.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

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T/K: \pm 3. x₁: \pm 8 % (relative error; compiler).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; (99685-96-81)	Scrivens, W.A.; Tour, J.M.
(2) Chlorobenzene; C ₆ H ₅ Cl; [108-90-7]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ^{•3})
22 7.9	x 10 ⁻³
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper.
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler), $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
(2) 1,2-Dibromobenzene; C ₆ H ₄ Br ₂ ; [583-53-9]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_{1}/(mol dm^{-3})$		
22 1.9	1.9×10^{-2}	
AUXILIARY	INFORMATION	
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler), c ₁ : ± 0.0007 mol dm ⁻³ .	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
(2) 1,3-Dibromobenzene; C ₆ H ₄ Br ₂ ; [108-36-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /	(mol dm ⁻³)	
22 1.9	1.9×10^{-2}	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 1,2-Dichlorobenzene; C₆H₄Cl₂; [95-50-1]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C x ₁		
22 5.3	x 10 ⁻⁵	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer. 	
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).	

Components:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
(2) 1,2-Dichlorobenzene; C ₆ H ₄ Cl ₂ ; [95-50-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_{1}/(mol dm^{-3})$		
22 3.4	3.41×10^{-2}	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid residue.	(2) Purity and chemical source were not given in the paper.	
	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.
[99685-96-8]	
<pre>(2) 1,3-Dichlorobenzene; C₆H₄Cl₂;</pre>	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207-
[541-73-1]	1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	

t/°C	$c_1/(mol dm^{-3})$
22	3.3×10^{-3}

AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi-	 Purity and chemical source were not given in the paper. Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS: $T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.



2,2'

ORIGINAL MEASUREMENTS:
Scrivens, W.A.; Tour, J.M. J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
PREPARED BY:
W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C

22

c ₁ /(m	ol	dm ⁻³)
1.44	x	10 ⁻²

AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper. 	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid residue.	(2) Purity and chemical source were not given in the paper.	
	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler), c ₁ : ± 0.0007 mol dm ⁻³ .	

234

23)

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Fluorobenzene; C₆H₅F; [462-06-6]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C x ₁		
22 7.8	3 x 10 ⁻⁵	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer. 	
	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Fluorobenzene; C₆H₅F; [462-06-6]</pre>	Scrivens, W.A.; Tour, J.M. J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207-	
	1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /	c ₁ /(mol dm ⁻³)	
22 1.7	1.7×10^{-3}	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(1) Purity and chemical source were not given in the paper.	
	(2) Purity and chemical source were not given in the paper.	
	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.	

COMPONENTS: ORIGINAL MEASUREMENTS: Scrivens, W.A.; Tour, J.M. Buckminsterfullerene; C₆₀; (99685-96-8) (2) Iodobenzene; C₆H₅I; [591-50-4] J. Chem. Soc., Chem. Commun. <u>1993</u>, 1207-1209. VARIABLES: PREPARED BY: T/K = Circa 295 (Ambient Room) W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C $c_1/(mol dm^{-3})$ 2.9×10^{-3} 22 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not Analytical balance and centrifuge. given in the paper. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for (2) Purity and chemical source were not given in the paper. about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue. ESTIMATED ERRORS: $T/K: \pm 3$ (Compiler). c₁: ± 0.0007 mol dm⁻³.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Buckminsterfullerene; C₆₀; [99685-96-8] 1-Bromo-2-methylnaphthalene; C₁₁H₉Br; [2586-62-1] 	Scrivens, W.A.; Tour, J.M. J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	

t/°C	c ₁ /(mol dm ⁻³)
22	4.83 x 10 ⁻²

AUXILIARY	INFORMATION
METROD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a $0.45 \ \mu\text{m}$ HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi-	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler), $c_1: \pm 0.0007 \text{ mol dm}^3$.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) 2-hydroxymethylbenzene; C ₇ n ₈ O; [95-48-7]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 2.9	x 10 ⁻⁶
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Carbon disulfide; CS₂; [75-15-0]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. <u>1992</u> , 57, 6077-6079.
VARIABLES:	PREPARED BY:
τ /κ = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	•

t/⁰C

30.0

7.16 x 10^{-3}

c₁/(mol dm⁻³)

AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectro- scopic grade n-hexane.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column. HPLC grade or AR grade solvent, chem- ical source not given, aromatic impuri- ties removed by chromatography if necessary. 	
	ESTIMATED ERRORS:	
	<pre>T/K: ± 0.1. c₁: ± 3 % (relative error; compiler).</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Carbon disulfide; CS₂; [75-15-0]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 6.6	x 10 ⁻⁴
AUXILIARY	INFORMATION
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec-	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 99 % (or better), chem- ical source not given, used as received from manufacturer.
tion at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS	OPTOTNAL MEASUREMENTS.
	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) Benzonitrile; $C_7 n_5 N$; [100-47-0]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	-
t/°C x ₁	
22 7.1	x 10 ⁻⁵
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:

 $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; [99685-96-8]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x1	
22 1.1	x 10 ⁻⁴
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) Pyridine; C₅H₅N; [110-86-1]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₁	
22 9.9	× 10 ⁻⁵
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, Baxter Scientific Pro- ducts, McGaw Park, Illinois, USA, was used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:

T/K: \pm 3. x₁: \pm 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C ₆₀ ;	Scrivens, W.A.; Tour, J.M.	
[99685-96-8] (2) Pyridine; C _{cHc} N; [110-86-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207-	
	1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /(mol dm ⁻³)	
22 4 x	10 ⁻⁴	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
Excess solute and solvent allowed to	(2) Purity and chemical source were not	
for 30 minutes. Solution centrifuged for	given in the paper.	
about 5 minutes and filtered through a $0.45 \ \mu m$ HPLC syringe filtered. Three		
1.0 mls were removed and placed in tared		
oil bath to facilitate solvent evapora-		
metrically from the weight of the solid		
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler) $c_1: \pm 0.0007 \text{ mol dm}^3.$	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; (99685-96-81)	Scrivens, W.A.; Tour, J.M.
(2) Quinoline; C ₉ H ₇ N; [91-22-5]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C C ₁ /	(mol dm ⁻³)
22 1.0	x 10 ⁻²
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	 Purity and chemical source were not given in the paper.
equilibrated in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C ₆₀ ; (99685-96-8)	Scrivens, W.A.; Tour, J.M.
(2) Thiophene; C ₄ H ₄ S; [110-02-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C	(mol dm ⁻³)
22 6 x	10-4
AUXILIARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
equilibrated in a room temperature bath for 30 minutes. Solution centrifuged for	(2) Purity and chemical source were not given in the paper.
about 5 minutes and filtered through a 0.45 μ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared	
vials, which were then placed in a heated oil bath to facilitate solvent evapora-	
tion. Concentrations determined gravi- metrically from the weight of the solid	
residue.	ESTIMATED ERRORS:
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$.
	1 -

COMPONENT S:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C₆₀; [99685-96-8] (2) 2-Methylthiophene; C₅H₆S; [554-14-3]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. <i>J. Phys. Chem.</i> <u>1993</u> , 97, 3379-3383.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₁		
22 9.1	x 10 ⁻⁴	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. Reagent grade, 98 % (or better), chem- ical source not given, used as received from manufacturer. 	
	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).	

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COMPONENTS: (1) Buckminsterfullerene; C ₆₀ ; [99685-96-8] (2) Tetrahydrothiophene; C ₄ H ₈ S; [110-01-0] VARIABLES:	ORIGINAL MEASUREMENTS: Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383. PREPARED BY:
T/K = Circa 295 (Ambient Room) EXPERIMENTAL VALUES	W.E. Acree, Jr.
t/°C x ₁ 22 3.6	x 10 ⁻⁶
METHOD: APPARATUS/PROCEDURE High performance liquid chromatograph system equipped with an ultraviolet detec- tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a	 SOURCE AND PURITY OF MATERIALS: (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry. (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K: \pm 3.$ $x_1: \pm 8$ % (relative error; compiler).
CARBAZOLE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

- A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>
 - n-hexane n-heptane n-octane n-decane n-hexadecane cyclohexane methylcyclohexane 2,2,4-trimethylpentane t-butylcyclohexane squalane decahydronaphthalene
- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene methylbenzene 1,4-dimethylbenzene chrysene 1,2,3,4-tetrahydronaphthalene

D. <u>Esters</u>

ethyl ethanoate butyl butyrate

E. Ethers

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

F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>

- trichloromethane tetrachloromethane 1-chlorohexane 1-chlorooctane thlorotetradecane chlorocyclohexane
- G. <u>Alcohols</u>

methanol ethanol 1,2-ethanediol

1-propanol 2-propanol 1-butanol 1-octanol phenol <u>Ketones</u> 2-propanone 2-butanone cyclohexanone acetophenone I. Miscellaneous Pure Solvents carbon disulfide pyridine quinoline thiophene dimethyl sulfoxide nitromethane acetic anhydride 1-methyl-2-pyrrolidinone N, N-dimethylacetamide N,N-dimethylformamide tetramethylene sulfone tributyl phosphate dibenzofuran

н.

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	McCargar, J.W.; Acree, W.E., Jr. Phys. Chem. Liq. <u>1987</u> , 17, 123-138.	
VARIABLES:	PREPARED BY:	
T/K ≈ 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.9999	0.000139	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimet thermometer, and an ultraviolet/visi spectrophotometer. Excess solute and solvent placed in	 amber (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol. (2) 99 %, Aldrich Chemical Company, was 	
glass bottles and allowed to equilib for several days at constant tempera Attainment of equilibrium verified b repetitive measurements. Aliquots of urated solutions transferred through coarse filter into tared volumetric flasks, weighed and diluted with met	rate stored over molecular sieves and dis- ture. tilled shortly before use. y sat- n a	
Concentrations determined spectropho metrically at 292 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1.5 $ % (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.	
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.	
VARIABLES:	PREPARED BY:	
<i>T</i> /K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x ₁	
25.0 0.9999	0.00017	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) ACS Reagent Grade, source not specified, was used as received.	
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). x_1 : \pm 3 % (relative error, compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	<i>x</i> ₁
25.0 0.9998	0.000173
AUXILIA	RY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol	(2) HPLC Grade, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	<i>*</i> 1
25.0 0.9998	0.00023
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into target volumetric	(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.

coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophoto-metrically at 292.5 nm.

ESTIMATED ERRORS:

T/K: \pm 0.1 (compiler). x₁: \pm 3 % (relative error, compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N;	[86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) n-Octane; C ₈ H ₁₈ ; [3	111-65-9]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	*2	×1
25.0	0.9998	0.000198
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	EDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature k thermometer, and an ul spectrophotometer.	oath, calorimetric ltraviolet/visible	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determine metrically at 292 nm.	ined spectrophoto-	ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.	
(2) n-Decane; C ₁₀ H ₂₂ ; [142-18-5]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x ₁	
25.0 0.9997	0.00029	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.	
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). x ₁ : \pm 3 % (relative error, compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.
(2) n-Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C x ₂	x 1
25.0 0.9997	0.00032
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was passed through a silica gel column.
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:
	T/K: \pm 0.1 (compiler). x ₁ : \pm 3 % (relative error, compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.	
(2) n-Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	J. Pharm. Sci. <u>1987</u> , 76, 572-574.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	<i>x</i> 1	
25.0 0.9996	0.000414	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-	(2) 99 %, Aldrich Chemical Company, was used as received.	
chloromethane. Concentrations determined spectrophotmetrically at 292 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 2$ % (relative error).	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [8	36-74-8]	Fung, HL.; Higuchi, T.
(2) n-Hexadecane; C ₁₆ H ₃₄ ;	[544-76-3]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		-
t/°C	*2	×1
25.0	0.9996	0.00059
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDU	IRE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bat thermometer, and an ultr spectrophotometer.	ch, calorimetric aviolet/visible	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.		(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.
Concentrations determine metrically at 292.5 nm.	d spectrophoto-	ESTIMATED ERRORS:
		$T/K: \pm 0.1$ (compiler). x ₁ : ± 3 % (relative error, compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-	7] Phys. Chem. Liq. <u>1987</u> , 17, 123-138.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x ₁
25.0 0.9	998 0.000183
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calo thermometer, and an ultraviolet spectrophotometer.	rimetric (1) 99 %, Aldrich Chemical Company, /visible Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.
Excess solute and solvent place glass bottles and allowed to eq for several days at constant te Attainment of equilibrium verif repetitive measurements. Aliquo urated solutions transferred th coarse filter into tared volume flasks, weighed and diluted wit	d in amber hilibrate mperature. Led by ts of sat- cough a tric n methanol. (2) HPLC Grade, 99.9 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. before use. Company as stored over molecular sieves and distilled shortly before use. before use. cough a tric
Concentrations determined spect. metrically at 292 nm.	Cophoto- ESTIMATED ERRORS:
	$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₁₀ N; [86-74-8] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
<i>T</i> /K = 293 and 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	<i>x</i> ₁
20.0 0.999+	0.000153
25.0 0.999+	0.000224
AUXII	LIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in clo glass container and allowed to equilibr for several hours at constant temperatu Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.05. x_i : \pm 3 \Im (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.	
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	x ₁	
25.0 0.9998	0.00018	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was distilled over phosphorous pent- oxide.	
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). x ₁ : \pm 3 % (relative error, compiler).	

COMPONENTS	OPTOINAL MEASUREMENTS.				
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.				
VARIABLES:	PREPARED BY:				
Temperature	W.E. Acree, Jr.				
EXPERIMENTAL VALUES					
т/к ×2	×1				
320.6 0.9993	0.00066				
321.1 0.9992	0.00083				
325.1 0.9989	0.00106				
357.2 0.9971	0.00293				
AUXILI	ARY INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slow increased. Solubility determined by	 (1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received. (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received. 				
noting the temperature at which the last trace of solid solute disappeared.	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003.				

COMPONENT S:	ORIGINAL MEASUREMENTS:			
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.			
<pre>(2) Methylcyclohexane; C₇H₁₄; [108-87-2]</pre>	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂	×1			
25.0 0.9998	0.000196			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric	 99%, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol. Gold Label, 99+%, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. 			
Concentrations determined spectrophoto-				
metrically at 292 nm.	ESTIMATED ERRORS:			
	$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).			

CONTROL STREET	ORTGINAL MEASUREMENTS				
CORFORMIS:					
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.				
(2) Cyclooctane; C ₈ H ₁₆ ; [292-64-8]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.				
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EXPERIMENTAL VALUES					
t/°C x ₂	x 1				
25.0 0.9997	0.000309				
AUXILIAR	Y INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.				
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.				
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:				
	$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).				

COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.				
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.				
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EIPERIMENTAL VALUES					
t/°C x ₂	×1				
25.0 0.9999	0.000126				
AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.				
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.				
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:				
	$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).				

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Carbazole; C ₁₂ H ₉ N; [86-7	4-8]	Fung, HL.; Higuchi, T.				
(2) 2,2,4-Trimethylpentane; [540-84-1]	с _{8^н18} ;	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t∕°C	x 2	x 1				
25.0	0.9998	0.00018				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.				
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.		(2) Reagent Grade, source not specified, was distilled over sodium.				
Concentrations determined s metrically at 292.5 nm.	pectrophoto-	ESTIMATED ERRORS:				
		$T/K: \pm 0.1$ (compiler). x: + 3 % (relative error, compiler).				

COMPONENTS :	ORIGINAL MEASUREMENTS:				
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	I ₉ N; [86-74-8] Anderson, B.D.				
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).				
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EXPERIMENTAL VALUES	-				
t/°C c ₁ /	(mol dm ⁻³)				
25.0 0.00077					
AUXILIARI					
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.				
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was stored over molecular sieves to remove trace water.				
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:				
	T/K: \pm 0.1 (compiler). c ₁ : \pm 3 % (relative error; compiler).				

COMPONENTS :	ORIGINAL MEASUREMENTS:							
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.							
(2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1]	J. Solution Chem. <u>1988</u> , 17, 1081-1091.					J. Solution Chem. <u>1968</u> , 17, 1081-1091.		
VARIABLES:	PREPARED BY:							
<i>T</i> /K = 298	W.E. Acree, Jr.							
EIPERIMENTAL VALUES	•							
t/°C x ₂	x ₁							
25.0 0.9997	0.000250							
AUXILIARY	INFORMATION							
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:							
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.							
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.							
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:							
	$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).							

COMPONENTS:	ORIGINAL MEASUREMENTS:			
 (1) Carbazole; C₁₂H₉N; [86-74-8] (2) 2,6,10,15,19,23-Hexamethyltetracosane (squalane); C₇₀H₄₂; [111-01-3] 	McCargar, J.W.; Acree, W.E., Jr. J. Pharm. Sci. <u>1987</u> , 76, 572-574.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES	1			
t/°C x ₂	× ₁			
25.0 0.9993	0.000671			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-	(2) 99 %, Aldrich Chemical Company, was used as received.			
chloromethane. Concentrations determined spectrophotmetrically at 292 nm.	ESTIMATED ERRORS:			
	$T/K: \pm 0.05.$ x ₁ : ± 2 % (relative error).			

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]		Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.				
<pre>(2) Decahydronaphthalene; C₁₀H₁₈; [91-17-8]</pre>		Fluid Phase Equilibr. <u>1989</u> , 44, 305-345.				
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
T/K	*2	x ₁				
333.3	0.9974	0.00263				
348.7	0.9959	0.00414				
357.6	0.9946	0.00544				
361.6	0.9944	0.00557				
376.0	0.9890	0.01098				
388.2	0.9812	0.01880				
402.2	0.9719	0.02811				
416.2	0.9503	0.04967				
438.2	0.9047	0.09527				
473.2	0.7009	0.29909				
491.7	0.4945	0.50551				
502.2	0.3085	0.69153				
AUXILIARY		INFORMATION				
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath a thermometer.	and a precision	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received				
Mixtures of known concentration glass ampoules and place temperature to equilibrate were rotated while bath tem increased. Solubility determines and the sol	ations sealed ed in constant . Samples mperature slowly rmined by	(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.				
noting the temperature at trace of solid solute disa	which the last	ESTIMATED ERRORS:				
		T/K: precision ± 0.1. $x_1: \pm 0.0003.$				

COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Carbazole; C ₁₂ H ₁₀ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.				
(2) Benzene; C ₆ H ₆ ; [71-43-2]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.				
VARIABLES:	PREPARED BY:				
T/K = 293 and 298	W.E. Acree, Jr.				
EXPERIMENTAL VALUES					
t/°C x ₂	× ₁				
20.0 0.996	0.00352				
25.0 0.996	0.00412				
AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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. 				
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: T/K: precision + 0.05.				
	$x_1: \pm 3$ % (relative error; compiler).				

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Benzene; C ₆ H ₆ ; [71-43-2]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.				
VARIABLES:			PREPARED F	3Y:		
Temperature	Temperature		W.E. Acree, Jr.			
EXPERIMENTAL V	ALUES		ļ			
T/K	x 2	×1	T/K	x2	×1	
307.1	0.9946	0.0054	326.8	0.9891	0.0109	
310.3	0.9932	0.0068	340.3	0.9866	0.0134	
313.2	0.9937	0.0063				
324.1	0.9907	0.0093				
		AUXILIARY	INFORMATION	ĩ		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE ANI	D PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.		 (1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received. 				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003.				

COMPONENTS:			ORIGINAL N	MEASUREMENTS:	1	
(1) Carbazole; C ₁₂ H ₁₀ N; [86-74-8] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3]		Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.				
VARIABLES:	VARIABLES:		PREPARED BY:			
T/K = 293, 313 and 333		W.E. Acree, Jr.				
EXPERIMENTAL	VALUES		[
t/°C	x 2	x 1	t/°C	x 2	<i>x</i> 1	
20.0	0.996	0.00374	60.0	0.989	0.0111	
40.0	0.993	0.00666				
		AUXILIARY	INFORMATIO	ท		
METHOD: APPARATUS/PROCEDURE Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.		 SOURCE AND PURITY OF MATERIALS: (1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %. (2) 99 %, Commercial sample, source and purification method was not specified. 				
		ESTIMATED ERRORS: T/K : precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).				

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) 1,4-Dimetryibenzene; C ₈ H ₁₀ ; [106-42-3]	32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	* ₁
20.0 0.995	0.00483
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliguots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:
	$x_1: \pm 3$ % (relative error; compiler).

COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669. (English translation)	
VARIABLES:	······································	PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES		•	
T/K	<i>x</i> 2	×1	
528.2	1.000	0.000	
519.7	0.903	0.097	
511.2	0.805	0.195	
500.7	0.698	0.302	
493.4	0.606	0.394	
482.9	0.505	0.495	
478.4	0.472	0.528	
477.2	0.445	0.555	
479.8	0.396	0.604	
484.7	0.347	0.653	
489.6	0.301	0.699	
499.2	0.200	0.800	
507.5	0.108	0.892	
517.2	0.000	1.000	
METHOD: APPARATUS/PROCEDUR	AUXILIARY	INFORMATION	
Phase diagram was determin thermal analysis method (d detail in V.M. Kravchenko, U.S.S.R. <u>1939</u> , 13, 133), visual observations.	ned using a described in , <i>J. Phys. Chem.</i> supplemented by	 (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use. ESTIMATED ERRORS: 	
		T/K: precision \pm 0.2 (Compiler). $x_1: \pm 0.002$ (Compiler).	

COMPONENTS:			ORIGINAL M	EASUREMENTS:	
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) 1,2,3,4-Tetrahydronaphthalene; C₁₀H₁₂; [119-64-2]</pre>		Coon, J.E Fluid Pha	2.; Auwaerter Ase Equilibr.	r, J.E.; McLaughlin, E. <u>1989</u> , 44, 305-345.	
VARIABLES:			PREPARED E	SY:	
Temperature			W.E. Acre	e, Jr.	
EXPERIMENTAL V	ALUES				
T/K	×2	*1	T/K	x2	×1
344.7	0.9927	0.0073	495.2	0.3029	0.6971
374.8	0.9897	0.0103			
476.2	0.7113	0.2887			
			SOURCE NUT		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(1) 99+ % wauke recei (2) 99.6+ store trace	Aldrich Ch e, Wisconsin ved. • %, Aldrich ed over molec water.	nemical Company, Mil- n, USA, was used as Chemical Company, was cular sieves to remove	
trace of soli	d solute dis	appeared.	<i>T/K:</i> prec x ₁ : ± 0.00	ision <u>+</u> 0.1.	

COMPONENTS	ARTAINAL MEASIDEMENTS.
COMPONENTS	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) Ethyl ethanoate; C,H.O.; [141-78-6]	Sov. Prog. Chem. 1986, 52, 41-44.
	(English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
-,	
······································	
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.980 0.0	20
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in	(1) Purity and chemical course not credi-
the paper.	fied in paper.
••	
Based upon experimental values given in	(2) Purity and chemical source not speci-
the paper for solvents for which indepen-	fied in paper.
estimates the temperature as between 298-	
303 K.	
	ESTIMATED EPROPS:
	T/K: Unknown.
	$x_1: \pm 8$ % (relative error; compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Carbazole; C₁₂H₉N; [86-74-8] Anderson, B.D. (2) Butyl butyrate; C₈H₁₆O₂; Ph.D. Dissertation, University of Kansas, [109-21-7] Lawrence, Kansas, USA (1978). VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EIPERIMENTAL VALUES $c_1/(\text{mol dm}^{-3})$ t/°C 25.0 0.0994 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer. (1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystal-lized from acetone-heptane mixtures. Excess solute and solvent placed in (2) Purity not given, Eastman Chemical Co., glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat-wated solutions transformed the Rochester, New York, USA, was shaken with sodium hydroxide, washed with distilled water, dried over magnesium sulfate and distilled. Stored over urated solutions transferred through a coarse filter into tared volumetric molecular sieves and distilled shortly before use. flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm. ESTIMATED ERRORS: T/K: \pm 0.1 (compiler). $c_1: \pm 3$ % (relative error; compiler).

COMPONENTS: (1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	ORIGINAL MEASUREMENTS: Acree, W.E., Jr.; McCargar, J.W.;	
(2) Tetrahydropyran; C ₅ H ₁₀ O; [142-68-7]	Phys. Chem. Liq. <u>1991</u> , 23, 27-35.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES	-	
t/°C x ₂	x 1	
25.0 0.9572	0.04284	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol. 99 %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. 	
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1: \pm 4$ % (relative error).	

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COMPONENTS :	UKIGINAL MEASUREMENIS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov	
(2) Tetrahydrofuran: C,H_O; [109-99-9]	Sov. Prog. Chem. <u>1986</u> , 52, 41-44.	
(2) 100101.julii	(English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.929 0.0	71	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 	
Based upon experimental values given in	(2) Purity and chemical source not speci-	
the paper for solvents for which indepen- dently determined values exist, compiler	fied in paper.	
estimates the temperature as between 298- 303 K.		
	ESTIMATED ERRORS:	
	T/K: Unknown.	
	$x_1: \pm 8$ % (relative error; compiler).	

COMPONENTS: (1) Carbazole; $C_{12}H_0N$; [86-74-8]	ORIGINAL MEASUREMENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,	
(2) 1,1-Oxybisethane; C ₄ H ₁₀ O; [60-29-7]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.987 0.03	13	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.
(2) 1,1-Oxybisethane; C ₄ H ₁₀ O; [60-29-7]	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	-
t/°C x ₂	×,
25.0 0.9870	0.0130
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was distilled from lithium aluminum hydride shortly before use.
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:
	T/K: \pm 0.1 (compiler). x_1 : \pm 3 % (relative error, compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.	
(2) 1,1-Oxybisbutane; C ₈ H ₁₈ O; [142-96-1]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.	
VARIABLES:	PREPARED BY:	
<i>T</i> /K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x1	
25.0 0.9950	0.005011	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).	

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	OPTOINT WEASIDEMENTS.	
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) 1,1 -Oxybisbutane; C₈H₁₈O; [142-96-1]</pre>	ORIGINAL MEASUREMENTS: Anderson, B.D. Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C C ₁ /	(mol dm ⁻³)	
25.0 0.0	287	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures. 	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99 %, Aldrich Chemical Company, was used as received.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	<pre>T/K: ± 0.1 (compiler). c₁: ± 3 % (relative error; compiler).</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Anderson, B.D.	
<pre>(2) 1,1 -Oxybispentane; C₁₀H₂₂O; [693-65-2]</pre>	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C c ₁		
25.0 0.0	182	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Purity not given, Pfaltz and Bauer, Waterbury, Connecticut, USA, was treated with potassium permanganate, washed with distilled water and sulfuric acid solution, dried over calcium chloride and distilled before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). c ₁ : \pm 3 % (relative error; compiler).	

COMPONENTS : ORIGINAL MEASUREMENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u>, 52, 41-44. (English Translation) (1) Carbazole; C₁₂H₉N; [86-74-8] (2) 1,4-Dioxane; C₄H₈O₂; [123-91-1] PREPARED BY: VARIABLES: T/K = See below W.E. Acree, Jr. EXPERIMENTAL VALUES x₂ x₁ 0.964 0.036 AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE (1) Purity and chemical source not speci-fied in paper. No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which indepen-dently determined values exist, compiler estimates the temperature as between 298-(2) Purity and chemical source not specified in paper. 303 K. ESTIMATED ERRORS: T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) Methoxybenzene; C₇H₈O; [100-66-3]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.987 0.03	13
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. x_1 : \pm 8 % (relative error; compiler).

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CORPORENTS I	URIGINAL MERSUREMENIS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.	
<pre>(2) Trichloromethane; CHCl₃; [67-66-3]</pre>	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.995	0.00478	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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. 	
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: T/K : precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Fung, HL.; Higuchi, T.	
<pre>(2) Trichloromethane; CHCl₃; [67-66-3]</pre>	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x ₂	<i>x</i> 1	
25.0 0.9963	0.0037	
AUXILIARY INFORMATION		
TEOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was washed with distilled water five times, stored overnight over calcium chloride and distilled from phosphorous pentoxide.	
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). x ₁ : \pm 3 % (relative error, compiler).	

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Carbazole; C₁₂H₀N; [86-74-8] Anderson, B.D. Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978). (2) Trichloromethane; CHCl₃; [67-66-3] VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(mol dm^{-3})$ t/°C 0.0468 25.0 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer. 99+ %, Aldrich Chemical Company, Mil-waukee, Wisconsin, USA, was recrystal-lized from acetone-heptane mixtures. Excess solute and solvent placed in (2) Purity not given, Fisher Scientific, glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat-Pittsburgh, Pennsylvania, USA, was washed with distilled water, stored over calcium chloride and distilled shortly before use. coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm. **ESTIMATED ERRORS:** $T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (relative error; compiler).

COMPONENTS :		ORIGINAL N	EASUREMENTS:		
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]		Smutek, M.; Fris, M.; Fohl, J.			
<pre>(2) Tetracloromethane; CCl₄; [56-23-5]</pre>		Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.			
VARIABLES:		PREPARED P	BY:		
T/K = 293, 298, 313 and 333		W.E. Acre	ee, Jr.		
EXPERIMENTAL VAL	UES				
t/°C	*2	×1	t/°C	*2	×1
20.0	0.999	0.000659	40.0	0.998	0.00165
25.0	0.999	0.000899	60.0	0.996	0.00377
AUXILIARY INFORMATION					
METHOD: APPARATU	S/PROCEDURE	8	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.		<pre>(1) coal sever pyric a fir (2) 99 %, purif</pre>	tar extract, cal times fro dine, and the hal purity of Commercial Eication meth	was recrystallized m toluene and n sublimed to give 98.3 %. sample, source and od was not specified.	
		ESTIMATED	ERRORS: cision ± 0.05		
		x ₁ : ± 3 %	(relative en	rror; compiler).	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₀ N; [86-74-8]		McCargar, J.W.; Acree, W.E., Jr.	
(2) 1-Chlorohexane; C ₆ H ₁₃ Cl; [544-10-5]		J. solution Chem. <u>1989</u> , 18, 151-158.	
VARIABLES: PREPARED		PREPARED BY:	
T/K = 298	B W.E. Acree, Jr.		
EXPERIMENTAL VALUES		1	
t∕°C	x 2	×1	
25.0	0.9974	0.00255	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCED	DURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bathermometer, and an ult spectrophotometer.	ath, calorimetric craviolet/visible	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.	
Concentrations determine metrically at 292 nm.	ned spectrophoto-	ESTIMATED ERRORS:	
		$T/K: \pm 0.05.$ x ₁ : ± 1.5 % (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H _g N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.	
(2) 1-Chlorooctane; C ₈ H ₁₇ Cl; [111-85-3]	J. Solution Chem. <u>1989</u> , 18, 151-158.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C x ₂	×1	
25.0 0.9976	0.00242	
AUXILIAR	Y INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Allouds of sat-	 (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol. (2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use. 	
urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:	
	$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).	

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Carbazole; C₁₂H_oN; [86-74-8] McCargar, J.W.; Acree, W.E., Jr. (2) 1-Chlorotetradecane; C14H20Cl; J. Solution Chem. <u>1989</u>, 18, 151-158. [2425-54-9] PREPARED BY: VARTABLES: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C x, x₁ 0.00240 0.9976 25.0 AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 3 times from absolute ethanol. Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate (2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of satbefore use. urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 292 nm.

$T/K: \pm 0.05.$ $x_1: \pm 1.5$ % (relative error).

ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.	
<pre>(2) Chlorocyclohexane; C₆H₁₁Cl; [542-18-7]</pre>	J. Solution Chem. <u>1989</u> , 18, 151-158.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES	-	
t/°C x ₂	<i>x</i> ₁	
25.0 0.9971	0.00291	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a	(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.	
coarse filter into tared volumetric flasks, weighed and diluted with methanol.		
coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Methanol; CH ₄ O; [67-56-1]	Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 293	W.E. Acree, Jr.	
EIPERIMENTAL VALUES	+	
t/°C x ₂	<i>*</i> 1	
20.0 0.998	0.00183	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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. 	
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.	
(2) Ethanol; C ₂ H ₆ O; [64-17-5]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.	
VARIABLES:	PREPARED BY:	
T/K = 293	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	×1	
20.0 0.997	0.00332	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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. 	
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.	
(2) Ethanol; C ₂ H ₆ O; [64-17-5]	Int. J. Pharm. <u>1994</u> , 104, 125-133.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	×1	
25.0 0.9964	0.00358	
AUXILIARY INFORMATION		
AZTHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and an ultraviolet/visible spectrophoto- meter.	(1) Purity and chemical source not given in paper.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.	(2) Purity and chemical source not given in paper.	
	ESTIMATED ERRORS:	
	T/K: \pm 0.2 (Compiler). x_1 : \pm 3 % (relative error, Compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Ethanol; C ₂ H ₆ O; [64-17-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
x ₂ x ₁	
0.9886 0.03	114
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) 1,2-Ethanediol; C ₂ H ₆ O ₂ ; [107-21-1]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	↓	
x ₂ x ₁		
0.993 0.0	07	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.
(2) 1-Propanol; C ₃ H ₈ O; [71-23-8]	Int. J. Pharm. <u>1994</u> , 104, 125-133.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x 1
25.0 0.9963	0.00365
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and an ultraviolet/visible spectrophoto- meter.	(1) Purity and chemical source not given in paper.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.	(2) Purity and chemical source not given in paper.
	ESTIMATED ERRORS:
	T/K: \pm 0.2 (Compiler). x ₁ : \pm 3 % (relative error, Compiler).

COMPONENTS:			ORIGINAL MEASUREMENTS: Smutek, M.; Fris, M.; Fohl, J. Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943. PREPARED BY:		
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) 2-Propanol; C ₃ H ₈ O; [67-63-0]					
VARIABLES:					
T/K = 293, 313 and 333		W.E. Acree, Jr.			
EXPERIMENTAL	VALUES				
t/°C	x 2	<i>x</i> 1	t/°C	×2	x 1
20.0	0.997	0.00277	60.0	0.991	0.00912
40.0	0.995	0.00523			
	<u></u>	AUXILIARY	INFORMATIO	'N	· · · · · · · · · · · · · · · · · · ·
METHOD: APPARATUS/PROCEDURE		SOURCE AN	D PURITY OF	MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.		<pre>(1) coal seve pyri a fi (2) 99 % puri</pre>	tar extract, ral times fro dine, and the nal purity of , Commercial fication meth	, was recrystallized om toluene and en sublimed to give f 98.3 %. sample, source and nod was not specified.	
		ESTIMATED	ERRORS :		

T/K: precision \pm 0.05. x₁: \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Anderson, B.D.	
(2) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
<i>T/</i> K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C c ₁ /	mol dm ⁻³)	
25.0 0.0493		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric	(2) puriss, 99.5 %, Fluka Chemical Corpora- tion, Ronkonkoma, New York, USA, was stored over molecular sieves to remove trace water.	

flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 356 nm. ESTIMATED ERRORS: T/K: \pm 0.1 (compiler). c₁: \pm 3 % (relative error; compiler).

COMPONENTES	OPTOINAL WEASIDEDENTS.
(1) Carbazole; C ₁₂ H ₉ N; [86~74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.
(2) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Int. J. Pharm. <u>1994</u> , 104, 125-133.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	×1
25.0 0.9956	0.00444
AUXILIARY	INFORMATION
	COURCE AND DUDTMY OF WAMEDIAL C.
METHOD: APPARATUS/PROCEDURE	SOURCE AND FURILI OF MATERIALS:
Constant temperature bath, thermometer, and an ultraviolet/visible spectrophoto- meter.	(1) Purity and chemical source not given in paper.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.	(2) Purity and chemical source not given in paper.
	ESTIMATED ERRORS:
	T/K: \pm 0.2 (Compiler). x_1 : \pm 3 % (relative error, Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Anderson, B.D.	
(2) 1-Octanol; C ₈ H ₁₈ O; [540-84-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C c ₁ /(/(mol dm ⁻³)	
25.0 0.0	0515	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). c_1 : \pm 3 % (relative error; compiler).	

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.	
(2) 1-Octanol; C ₈ H ₁₈ O; [540-84-1]	Int. J. Pharm. <u>1994</u> , 104, 125-133.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x ₂	x 1	
25.0 0.9919	0.00806	
AUXILIARY	INFORMATION	
METROD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and an ultraviolet/visible spectrophoto- meter.	(1) Purity and chemical source not given in paper.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.	(2) Purity and chemical source not given in paper.	
	ESTIMATED ERRORS:	
	T/K: \pm 0.2 (Compiler). $x_1: \pm 3$ % (relative error, Compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) Phenol; C ₆ H ₆ O; [108-95-2]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 313	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	x ₁
40.0 0.994	0.00598
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: T/K: precision + 0.05.
	$x_1: \pm 3$ % (relative error; compiler).

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CORPORENTS:	ORIGINAL MEASUREMENIS:		
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.		
(2) 2-P ropanon e ; C ₃ H ₆ O; [67-64-1]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.		
VARIABLES:	PREPARED BY:		
T/K = 293	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x ₂	<i>x</i> 1		
20.0 0.976	0.0239		
AUIILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 (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. 		
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:		
	T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).		

COMPONENTS: (1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) 2-Propanone; C ₃ H ₆ O; [67-64-1] VARIABLES: T/K = See below	ORIGINAL MEASUREMENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation) PREPARED BY: W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.9628 0.0	372
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. x ₁ : <u>+</u> 8 % (relative error; compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u>, 52, 41-44. (English Translation) (1) Carbazole; C₁₂H₀N; [86-74-8] (2) 2-Butanone; C₄H₈O; [78-93-3] PREPARED BY: VARIABLES: T/K = See below W.E. Acree, Jr. EXPERIMENTAL VALUES x2 x₁ 0.9576 0.0424 AUXILIARY INFORMATION METROD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source not speci-fied in paper. No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which indepen-dently determined values exist, compiler estimates the temperature as between 298-(2) Purity and chemical source not speci-fied in paper. 303 K. ESTIMATED ERRORS:

T/K: Unknown.

 $x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) Cycloberanone: C H .O: (108=94=1)	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986 52. Al-AA
(2) cyclonexatione, $c_{6n_{10}}$, $(100.54.1)$	(English Translation)
VARTABLES:	PREPARED BY:
T/K ≖ See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.932 0.0	68
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
<pre>(2) Carbon disulfide; CS₂; [75-15-0]</pre>	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
T /K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x ₂	×1
20.0 0.999	0.00149
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature.	 (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
Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remayned	purification method was not specified.
after solvent had evaporated.	ESTIMATED ERRORS:
	T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

COMPONENTS:			ORIGINAL MEASUREMENTS:					
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]			Smutek, M.; Fris, M.; Fohl, J.					
(2) Pyridine; C ₅ H ₅ N; [110-86-1] VARIABLES:			Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943. PREPARED BY:					
								T/K = 293, 313 and 333
EXPERIMENTAL VAL	LUES		•					
t/°C	<i>x</i> 2	* 1	t/°C	x 2	x 1			
20.0	0.911	0.0895	60.0	0.862	0.138			
40.0	0.890	0.110						
AUXILIARY INFORMATION								
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:					
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.			 (1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %. (2) 99 %, Commercial sample, source and purification method was not specified. 					
			ESTIMATED ERRORS:					
			T/K: precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).					

COMPONENTS: (1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Pyridine; C ₅ H ₅ N; [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			W.E. Acree, Jr.					
EXPERIMENTAL V	ALUES							
T/K	×2	<i>*</i> 1	T/K	×2	<i>x</i> 1			
301.5	0.9023	0.0977	400.7	0.7376	0.2624			
318.1	0.8852	0.1148	439.2	0.6167	0.3833			
345.5	0.8510	0.1490						
370.3	0.8041	0.1959						
AUXILIARY INFORMATION								
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:					
Constant temperature bath and a precision thermometer.			(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received.					
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.					
			ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003.					
COMPONENTS	OBTOTUNT WENCIDENTE							
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	ORIGINAL MEASUREMENTS:							
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,							
(2) Pyridine; C ₅ H ₅ N; [110-86-1]	Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)							
VARIABLES:	PREPARED BY:							
T/K = See below	W.E. Acree, Jr.							
EIPERIMENTAL VALUES								
x ₂ x ₁								
0.914 0.04	86							
AUXILIARY	INFORMATION							
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:							
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 							
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.							
	ESTIMATED ERRORS:							
	T/K: Unknown. x_1 : \pm 8 % (relative error; compiler).							

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) Quinoline; C₉H₇N; [91-22-5]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
x ₂ x ₁		
0.879 0.121		
AUIILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical Source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Thiophene; C ₄ H ₄ S; [110-02-1]	Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. 1988, 16, 519-534.
	21 201 2020 Chemi 2000, 10, 515 554.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
T/K ×2	x ₁
313.7 0.9893	0.0107
337.1 0.9796	0.0204
345.6 0.9746	0.0254
349.5 0.9713	0.0287 .
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	<pre>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</pre>
noting the temperature at which the last	ESTIMATED ERRORS:
trace of solid solute disappeared.	T/K: precision <u>+</u> 0.1. x ₁ : <u>+</u> 0.0003.

COMPONENTS: (1) Carbazole; C ₁₂ H ₉ N; [86-74-8] (2) Dimethylsulfoxide; C ₂ H ₆ OS; [67-68-5] VARIABLES: T/K = See below	ORIGINAL MEASUREMENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation) PREPARED BY: W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.861 0.13	39	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) Nitromethane; CH ₂ NO ₂ ; [75-52-5]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44.
(-)	(English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	I
x ₂ x ₁	
0.996 0.00	D4
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).

	OBTOINAL MEASUREMENTS.	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	CRIGINAL MEASUREMENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44.	
[108-24-7]	(English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.988 0.03	12	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. x_1 : ± 8 % (relative error; compiler).	

	*
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) 1-Methyl-2-pyrrolidinone; C₅H₉NO; [872-50-4]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. <i>Sov. Prog. Chem.</i> <u>1986</u> , <i>52</i> , 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x ₂ x ₁	
0.843 0.1	57
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	$x_1: \pm 8$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.	
<pre>(2) N,N-Dimethylacetamide; C₂H₉NO; [127-19-5]</pre>	Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.810 0.19	90	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8 $ (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) N,N-Dimethylformamide; C₃H₇NO; [68-12-2]</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
x ₂ x ₁		
0.836 0.1	64	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
 (1) Carbazole; C₁₂H₉N; [86-74-8] (2) Tetramethylene sulfone; C₄H₈O₂S; [126-33-0] 	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.9526 0.0474		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	 Purity and chemical source not speci- fied in paper. 	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. x_1 : \pm 8 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Carbazole; C₁₂H₉N; [86-74-8] (2) Tributyl phosphate; C₁₂H₂₇O₄P; [126-73-8] VARIABLES:</pre>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation) PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x ₂ x ₁		
0.911 0.089		
AUXILIARY	INFORMATION	
METEOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1: \pm 8$ % (relative error; compiler).	

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COMPONENTS :	ORIGINAL MEAS	SUREMENTS:
(1) Carbazole; C ₁₂ H ₉ N; [86-74-8]	Cullinane, 1	N.M.; Rees, W.T.
(2) Dibenzofuran; C ₁₂ H ₈ O; [132-64-9]	Trans. Farad	day Soc. <u>1940</u> , 36, 506-514.
VARIABLES:	PREPARED BY:	<u> </u>
Temperature	W.E. Acree,	Jr.
EXPERIMENTAL VALUES ^a	·····	
T _{io} /K T _{tio} /K	x 2	x 1
355.6 354.7	1.000	0.000
401.6 356.7	0.898	0.102
439.2 360.7	0.753	0.247
469.5 368.6	0.562	0.438
492.8 382.7	0.331	0.669
510.0	0 141	0.859
510.0 510.2	0.141	1,000
AUXILI	ARY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PT	URITY OF MATERIALS:
Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported tempera- tures verified by repetitive measurement	(1) Purity a was subl acetone (2) Purity a s. in paper lized fr	and chemical source not given, limed and recrystallized from and chemical source not given r, was sublimed and recrystal- com alcohol several times.
	ESTIMATED ERF T/K: precisi $x_1: \pm 0.002$	RORS: Lon <u>+</u> 0.2 (Compiler). (Compiler).

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CHRYSENE SOLUB	ILITIES IN PURE AND BINARY SOLVENT MIXTURES
А.	Saturated_Hydrocarbons (including_cycloalkanes)
	n-heptane
в.	Alkenes
с.	Aromatic_Hydrocarbons
	benzene
	naphthalene
	anthracene
	benz[a]anthracene
	acenaphthene
	fluorene
	b) reve
D.	Esters
Ε.	Ethers
F.	Haloalkanes and Haloaromatic Hydrocarbons
G.	Alcohols
	1-octanol
н.	Ketones
Ι.	<u>Miscellaneous Pure Solvents</u>
	carbazole
	dibenzofuran
J.	Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Chrysene; C₁₈H₁₂; [218-01-9] (2) n-Heptane; C₇H₁₆; [142-82-5]</pre>	Lissi, E.A.; Abuin, E.B. Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C c ₁ /	(mol dm ⁻³)
20.0 0.0	040
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, centrifuge, thermometer, and an uv/visible spectro- photometer.	(1) Purity not given, commercial sample of unspecified source, was used as received.
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the mea- sured absorbance using the Beer-Lambert law.	(2) Purity and chemical source not given, purification procedure not specified.
	ESTIMATED ERRORS:
	$T/K: \pm 2.$ $c_1:$ unknown.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		McLaughlin, E.; Zainal, H.A.		
(2) Benzene; C ₆ H ₆ ; [71-43-2	2]	J. Chem. Soc. <u>1959</u> , 863-867.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
<i>T/</i> K	*2	*1		
308.8	0.9979	0.0021		
319.0	0.9968	0.0032		
333.8	0.9948	0.0052		
345.4	0.9921	0.0079		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.		(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with toluene eluant.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) "AnalaR", was dried over sodium wire and freshly distilled before use.		
noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003 (compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Proc. Acad. Sci. U.S.S.R., Sect. Chem. <u>1956</u> , 111, 667-669 (English translation)	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	×2	×1	
353.2	1.000	0.000	
351.7	0.975	0.025	
351.0	0.958	0.042	
388.4	0.897	0.103	
406.2	0.843	0.157	
417.8	0.798	0.202	
442.4	0.710	0.290	
459.7	0.593	0.407	
476.2	0.496	0.504	
487.5	0.407	0.593	
500.2	0.298	0.702	
511.4	0.183	0.817	
520.2	0.097	0.903	
528.2	0.000	1.000	
AUXILIARY INFORMATION		INFORMATION	
METEOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
thermal analysis method (deso detail in V.M. Kravchenko, J. U.S.S.R. <u>1939</u> , 13, 133), su	using a cribed in . Phys. Chem. oplemented by	(1) Furity and chemical source were not specified in paper, was recrystallized before use.	
visual observations.	-	(2) Purity and chemical source were not specified in paper, was recrystallized before use.	
	ļ	ESTIMATED ERRORS:	
		T/K: precision \pm 0.2 (Compiler). $x_1: \pm 0.002$ (Compiler).	
		<u> </u>	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		Proc. Acad. Sci. U.S.S.R., Sect. Chem. <u>1956</u> , 111, 667-669 (English translation)	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES		•	
T/K	×2	×1	
489.7	1.000	0.000	
481.7	0.897	0.103	
473.7	0.798	0.202	
469.7	0.740	0.260	
467.2	0.697	0.303	
466.2	0.635	0.365	
470.5	0.598	0.402	
480.4	0.504	0.496	
490.9	0.397	0.603	
499.7	0.307	0.693	
509.5	0.212	0.788	
519.2	0.104	0.896	
528.2	0.000	1.000	
AUXILIARY INFORMATION		INFORMATION	
METHOD: APPARATUS/PROCEDURE	tuging -	SOURCE AND PURITY OF MATERIALS:	
thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. <u>1939</u> , 13, 133), supplemented by visual observations.		 (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use. ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x₁: ± 0.002 (Compiler). 	
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COMPONENTS:		
	ORIGINAL MEASUREMENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	Sturrock, M.G.; Lawe, T.	
(2) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3]	Can. J. Re	s., Sect. B. <u>1939</u> , 17, 71-74.
VARIABLES:	PREPARED BY	:
Temperature	W.E. Acree	, Jr.
EXPERIMENTAL VALUES ^a	ļ	
T_{in}/K T_{fin}/K	^x 2	×1
433.2 433.2	1.00	0.00
448.2 436.2	0.90	0.10
470.2 442.2	0.75	0.25
487.2 451.2	0.60	0.40
496.2 461.2	0.50	0.50
505.2 468.2	0.40	0.60
516.2 484.2	0.25	0.75
525.2 505.2	0.10	0.90
528.2 528.2	0.00	1.00
AUTILIARY	INFORMATION	
AUXILIARY METHOD: APPARATUS/PROCEDURE	INFORMATION SOURCE AND B	PURITY OF MATERIALS:

COMPONENTS:	ORIGINAL MEA	SUREMENTS:		
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	Kravchenko, V.M.; Pastukhova, I.S.			
(2) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3]	Proc. Acad. <u>1956</u> , 111,	Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)		
VARIABLES:	PREPARED BY:			
Temperature	W.E. Acree,	Jr.		
EXPERIMENTAL VALUES ^a				
T_{in}/K T_{fin}/K	*2	×1		
431.2 430.9	1.000	0.000		
435.4 431.7	0.960	0.040		
438.2 432.2	0.947	0.053		
446.7 434.2	0.898	0.102		
451.6 436.2	0.852	0.148		
459.2 438.6	0.805	0.195		
473.8 445.2	0.700	0.300		
483.2 453.2	0,603	0.397		
403.7 455.2	0.498	0.502		
502 2 474 2	0 395	0.605		
	0.395	0.300		
508.7 400.2	0.300	0.700		
514.5 499.2	0.202	0.798		
522.2 513.2	0.095	0.905		
which crystallization begins; crystallization of the solid g	fin is the tempe olution conclude	erature at which		
AUXILIAR	Y INFORMATION	-		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PU	RITY OF MATERIALS:		
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. <u>1939</u> , 13, 133), supplemented by	(1) Purity a specifie before u	nd chemical source were not d in paper, was recrystallized se.		
visual observations.	(2) Purity and chemical source were not specified in paper, was recrystallized before use.			
	ESTIMATED ERR	ORS:		
	T/K: precision x_1 : \pm 0.002	on <u>+</u> 0.2 (Compiler). (Compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]		Proc. Acad. Sci. U.S.S.R., Sect. Chem. <u>1956</u> , 111, 667-669 (English translation)	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	*2	x1	
368.2	1.000	0.000	
366.4	0.966	0.034	
364.2	0.928	0.072	
378.5	0.899	0.101	
416.2	0.796	0.204	
437.4	0.704	0.296	
457.0	0.596	0.404	
471.5	0.499	0.501	
477.8	0.387	0.613	
500.2	0.278	0.722	
513.2	0.147	0.853	
528.2	0.000	1.000	
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Phase diagram was determined thermal analysis method (des detail in V.M. Kravchenko, J U.S.S.R. 1939, 13, 133), su	using a cribed in . Phys. Chem. pplemented by	 Purity and chemical source were not specified in paper, was recrystallized before use. 	
visual observations.	*	(2) Purity and chemical source were not specified in paper, was recrystallized before use.	
	Ī	ESTIMATED ERRORS:	
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).	
		<u> </u>	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		Kravchenko, V.M.; Pastukhova, I.S.
(2) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]		Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
T/K	*2	<i>x</i> ₁
387.2	1.000	0.000
384.4	0.948	0.052
381.2	0.902	0.098
395.7	0.871	0.129
419.5	0.795	0.205
445.4	0.680	0.320
458.7	0.597	0.403
480.2	0.445	0.555
491.6	0.350	0.650
504.2	0.246	0.754
513.9	0.139	0.861
528.2	0.000	1.000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Phase diagram was determined thermal analysis method (des detail in V.M. Kravchenko, J U.S.S. 133, 133), su	using a cribed in 7. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.
visual observations.	Francisca pl	(2) Purity and chemical source were not specified in paper, was recrystallized before use.
		ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x ₁ : \pm 0.002 (Compiler).
		<u> </u>

ENTS :		

ORIGINAL MEASUREMENTS: COMPONE (1) Chrysene; C₁₈H₁₂; [218-01-9] Kravchenko, V.M.; Pastukhova, I.S. Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation) (2) Fluoranthene; C₁₆H₁₀; [206-44-0] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K x₂ **x**1 0.000 383.2 1.000 378.7 0.939 0.061 378.2 0.918 0.082 387.3 0.897 0.103 403.2 0.846 0.154 418.8 0.799 0.201 442.4 0.691 0.309 457.2 0.602 0.398 474.5 0.498 0.502 486.2 0.404 0.596 498.4 0.293 0.707 510.5 0.195 0.805 519.2 0.090 0.910 528.2 0.000 1.000 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Phase diagram was determined using a

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

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

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

ESTIMATED ERRORS:

T/K: precision \pm 0.2 (Compiler). x₁: \pm 0.002 (Compiler).

Components:		ORIGINAL MEASUREMENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) Pyrene; C ₁₆ H ₁₀ ; [129-00-	-0]	Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES		•	
T/K	*2	x ₁	
423.2	1.000	0.000	
413.7	0.901	0.099	
410.2	0.864	0.136	
408.2	0.835	0.165	
415.4	0.813	0.187	
420.6	0.790	0.210	
441.2	0.697	0.303	
458.7	0.602	0.398	
473.2	0.505	0.495	
487.2	0.396	0.604	
496.2	0.314	0.686	
506.7	0.218	0.782	
517.7	0.103	0.897	
528.2	0.000	1.000	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	·····	SOURCE AND PURITY OF MATERIALS:	
Phase diagram was determine thermal analysis method (de detail in V.M. Kravchenko,	d using a scribed in J. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.	
visual observations.	арртешенска ру	(2) Purity and chemical source were not specified in paper, was recrystallized before use.	
		ESTIMATED ERRORS:	
		T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).	
		l	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] (2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. <i>Environ. Sci. Technol.</i> <u>1985</u> , 19, 522-529.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C c ₁ /0	(mol dm ⁻³)	
25.0 0.00	0200	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection.	 Highest available commercial purity, specific chemical supplier not given, was used as received. 	
Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 %	(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.	
SE30 ultraphase column.	ESTIMATED ERRORS:	
	T/K: \pm 0.1 (compiler). c_1 : \pm 3 % (relative error; compiler).	

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COMPONENTS:		ORIGINAL MEASUREMENTS:
<pre>(1) Chrysene; C₁₈H₁₂; [218-01-9] (2) Carbazole; C₁₂H₉N; [86-74-8] VARIABLES:</pre>		Kravchenko, V.M.; Pastukhova, I.S.
		Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)
		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		•
т/к	x2	<i>x</i> 1
517.2	1.000	0.000
507.5	0.892	0.108
499.2	0.800	0.200
489.6	0.699	0.301
484.7	0.653	0.347
479.8	0.604	0.396
477.2	0.555	0.445
478.4	0.528	0.472
482.9	0.495	0.505
493.4	0.394	0.606
500 7	0.302	0.698
511.2	0.195	0.805
519.7	0.097	0.803
517.7	0.000	1,000
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Phase diagram was determin thermal analysis method (d detail in V.M. Kravchenko, U.S.S.R. 1939. 13. 133).	ed using a escribed in J. Phys. Chem. supplemented by	 (1) Purity and chemical source were not specified in paper, was recrystallized before use.
visual observations.		(2) Purity and chemical source were not specified in paper, was recrystallized before use.
		ESTIMATED ERRORS:
		T/K: precision \pm 0.2 (Compiler). x ₁ : \pm 0.002 (Compiler).

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COMPONENTS:	
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	
(2) Dibenzofuran; C ₁₂ H ₈ O; [132-64-9]	

ORIGINAL MEASUREMENTS:

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

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

VARIABLES:

Temperature

T/K	*2	x 1
356.2	1.000	0.000
354.7	0.968	0.032
353.2	0.940	0.060
373.7	0.907	0.093
401.2	0.848	0.152
429.2	0.752	0.248
450.4	0.649	0.351
474.6	0.496	0.504
486.7	0.404	0.596
499.0	0.300	0.700
509.6	0.295	0.805
516.5	0.113	0.887
528.2	0.000	1.000

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

CORONENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

n-heptane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons
- D. <u>Esters</u>
- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. <u>Alcohols</u>

1-octanol

- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Coronene; C ₂₄ H ₁₂ ; [191-07-1]	Lissi, E.A.; Abuin, E.B.	
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.	
VARIABLES:	PREPARED BY:	
<i>T</i> /K = 293	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$t/^{\circ}C$ $c_1/(mol dm^{-3})$		
20.0 0.00048		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.	
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the mea- sured fluorescence emission intensity.	(2) Purity and chemical source not given, purification procedure not specified.	
	ESTIMATED ERRORS:	
	<i>T/K</i> : <u>+</u> 2. C ₁ : unknown.	
	•	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 Coronene; C₂₄H₁₂; [191-07-1] 1-Octanol; C₈H₁₈O; [111-87-5] 	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. <i>Environ. Sci. Technol.</i> <u>1985</u> , 19, 522-529.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	c ₁ /(mol dm ⁻³)	
25.0	0.000386	
AUXILIARY INFORMATION		

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection.	 Highest available commercial purity, specific chemical supplier not given, was used as received.
Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 a	(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
SE30 ultraphase column.	ESTIMATED ERRORS: $T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (relative error; compiler).
	$c_1: \pm 3$ % (relative error; compiler).

DIBENZ[a,h]ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

n-heptane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons
- D. <u>Esters</u>
- E. <u>Ethers</u>
- F. <u>Haloalkanes_and_Haloaromatic_Hydrocarbons</u>
- G. Alcohols

1-octanol

- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; (53-70-3)	Lissi, E.A.; Abuin, E.B.	
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.	
VARIABLES:	PREPARED BY:	
T/K = 293	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-	
t/°C	mol dm ⁻³)	
20.0 0.00034		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and an uv/visible spectro- photometer.	 Purity not given, commercial sample of unspecified source, was used as received. 	
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the mea- sured absorbance using the Beer-Lambert law.	(2) Purity and chemical source not given, purification procedure not specified.	
	ESTIMATED ERRORS:	
	$T/K: \pm 2.$ $c_1:$ unknown.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Dibenz[a,h]anthracene; C₂₂H₁₄; [53-70-3] (2) 1-Octanol; C₈H₁₈O; [111-87-5]</pre>	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. <i>Environ. Sci. Technol.</i> <u>1985</u> , 19, 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	

t/°C		
25.0		

 $c_1/(mol dm^{-3})$

0.000938

AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and a gas-liquid chromato- graph with flame ionization detection.	 Highest available commercial purity, specific chemical supplier not given, was used as received. 	
Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before anal- ysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.	(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.	
	ESTIMATED ERRORS: $T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (relative error; compiler).	

DIBENZOFURAN SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane decahydronaphthalene

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene 1,2,3,4-tetrahydronaphthalene

- D. <u>Esters</u>
- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. <u>Alcohols</u>
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>

pyridine thiophene

J. Binary Solvent Mixtures

2	n	A
J	υ	4

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C ₁₂ H ₈ O; [132-64-9] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.				
VARIABLES:			PREPARED E	3¥:	·····	
Temperature		W.E. Acre	ee, Jr.			
EXPERIMENTAL	VALUES					
T/K	x 2	x 1	T/K	x 2	×1	
327.8	0.5774	0.4226	338.5	0.3300	0.6700	
330.2	0.5195	0.4805	345.1	0.1880	0.8120	
334.0	0.4564	0.5436				
337.5	0.3700	0.6300				
		AUXILIARY	INFORMATION	ł		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly		(1) 99 %, kee, from (2) Gold Compa	Aldrich Che Wisconsin, U toluene. Label, 99.9+ any, was used	mical Company, Milwau- SA, was recrystallized %, Aldrich Chemical as received.		
noting the te trace of soli	emperature at Ld solute disa	which the last appeared.	ESTIMATED T/K: prec $x_1: \pm 0.0$	ERRORS: cision <u>+</u> 0.1. 003.		

COMPONENTS:			ORIGINAL M	EASUREMENTS:	
 (1) Dibenzofuran; C₁₂H₈O; [132-64-9] (2) Decahydronaphthalene; C₁₀H₁₈; [91-17-8] 			Coon, J.E Fluid Pha	5.; Auwaerter Ase Equilibr.	;, J.E.; McLaughlin, E. . <u>1989</u> , 44, 305-345.
VARIABLES:		· · · · · · · · · · · · · · · · · · ·	PREPARED B	Y:	
Temperature			W.E. Acree, Jr.		
EXPERIMENTAL V	ALUES		Į		
T/K	x 2	x 1	T/K	x 2	x 1
326.4	0.5755	0.4245	337.2	0.3553	0.6447
328.2	0.5354	0.4646			
331.5	0.4890	0.5110			
333.5	0.4248	0.5752			
		AUXILIARY	INFORMATION	I	
METHOD: APPARA	TUS/PROCEDURI	5	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.			(1) 99.6 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from solution.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.			
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			ESTIMATED <i>T/K</i> : prec <i>x</i> ₁ : ± 0.00	ERRORS: fision <u>+</u> 0.1. 003.	

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Dibenzofuran; C ₁₂ H	I ₈ 0; [132-64-9]	Domanska, U.; Groves, F.R., Jr.; McLaughlin, E.		
(2) Benzene; C ₆ H ₆ ; [7]	-43-2]	J. Chem. Eng. Data <u>1993</u> , 38, 88-94.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	*2	×1		
278.7	1.0000	0.0000		
276.1	0.9365	0.0635		
274.0	0.9144	0.0856		
273.4	0.9066	0.0934		
272.4	0.8878	0.1122		
274.8	0.8761	0.1239		
277.9	0.8637	0.1363		
280.2	0.8537	0.1463		
282.8	0.8401	0.1599		
290.3	0.8022	0.1978		
296.3	0.7654	0.2346		
298.3	0.7520	0.2480		
302.5	0.7187	0.2813		
305.3	0.7005	0.2995		
312.0	0.6441	0.3559		
320.0	0.5514	0.4486		
329.1	0.4209	0.5791		
337.7	0.2955	0.7045		
340.9	0.2430	0.7570		
346.4	0.1654	0.8346		
355.3	0.0000	1.0000		
1				
	AUXILIARY	TNFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature h thermometer.	bath and a precision	 (1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene. 		
in glass ampoules and temperature to equilib were rotated while bat increased. Solubility	placed in constant prate. Samples th temperature slowly determined by	(2) 99+ %, Aldrich Chemical Company, was fractionally distilled and stored over molecular sieves.		
noting the temperature trace of solid solute	at which the last disappeared.	ESTIMATED ERRORS:		
		T/K: precision ± 0.1. $x_1: \pm 0.0003.$		
· · · · · · · · · · · · · · · · · · ·				

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C ₁₂ H ₈ O; [132-64-9] (2) Benzene; C ₆ H ₆ ; [71-43-2]			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.			
VARIABLES:			PREPARED BY	:		
Temperature			W.E. Acree	, Jr.		
EXPERIMENTAL V	VALUES		.			
T/K	*2	×1	T/K	x2	×1	
321.9	0.5203	0.4797	338.7	0.2776	0.7224	
323.5	0.4932	0.5068				
329.4	0.4156	0.5844				
332.0	0.3778	0.6222				
		AUXILIARY	INFORMATION			
METHOD: APPARI	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.			 (1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene. 			
in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the te trace of soli	increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			RRORS: sion <u>+</u> 0.1. D3.		

COMPONENTS:			ORIGINAL A	PASUREMENTS:		
CONTRACTOR			UNIGINIE -			
(1) Dibenzofuran; C ₁₂ H ₈ O; [132-64-9]			Coon, J.H	3.; Auwaerter	, J.E.; McLaughlin, E.	
(2) 1,2,3,4-Tetrahydronaphthalene; C ₁₀ H ₁₂ ; [119-64-2]			Fluid Pha	ase Equilibr.	<u>1989</u> , <i>44</i> , 305-345.	
VARIABLES:			PREPARED F	3Y:		
Temperature	Temperature			W.E. Acree, Jr.		
EXPERIMENTAL V	VALUES		1			
T/K	×2	<i>x</i> 1	T/K	*2	×1	
318.9	0.5479	0.4521	339.5	0.2670	0.7330	
322.6	0.5093	0.4907				
326.6	0.4506	0.5494				
337.9	0.3010	0.6990				
		AUXILIARY	INFORMATION			
METHOD: APPARA	TUS/PROCEDURE	s	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temp thermometer.	Constant temperature bath and a precision thermometer.			(1) 99.6 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- from solution.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.			
noting the te	mperature at	which the last	ESTIMATED	ERRORS:		
trace of soli	d solute disa.	ppeared.	<i>T/K</i> : prec <i>x</i> ₁ : <u>+</u> 0.04	ision <u>+</u> 0.1. 003.		

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C ₁₂ H ₈ O; [132-64-9]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.				
(2) Pyridine;	; C5H5N; [110-	-00-1]	J. Soluti	on Chem. <u>19</u>	<u>88</u> , <i>16</i> , 519-534.	
VARIABLES:			PREPARED B	Y:		
Temperature			W.E. Acre	e, Jr.		
EXPERIMENTAL V	VALUES		1			
T/K	*2	×1	T/K	*2	* ₁	
323.7	0.4917	0.5083	340.8	0.2418	0.7582	
326.2	0.4554	0.5446				
331.2	0.3839	0.6161				
336.3	0.3188	0.6812				
		AUXILIARY	INFORMATION	ı		
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.			(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
		abboared.	T/K : precision \pm 0.1. x_1 : \pm 0.0003.			

COMPONENT S:			ORIGINAL MEASUREMENTS:				
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.					
(2) Thiophene; C_4H_4S ; [110-02-1]			J. Soluti	on Chem. <u>198</u>	<u>38</u> , <i>16</i> , 519-534.		
VARIABLES:	VARIABLES:			PREPARED BY:			
Temperature			W.E. Acre	e, Jr.			
EXPERIMENTAL V	ALUES						
T/K	x2	×1	т/ К	*2	×1		
314.2	0.5780	0.4220	337.0	0.3040	0.6960		
319.3	0.5243	0.4757	341.1	0.2415	0.7585		
322.3	0.4917	0.5083					
332.8	0.3653	0.6347					
		AUXILIARY	INFORMATION	r			
METHOD: APPARA	TUS/PROCEDURE	6	SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed			 (1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene. (2) Table Lobel 20 and all his chemical company. 				
in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the ter	mperature at	which the last	ESTIMATED	ERRORS:			
		ppeared.	$T/K:$ precision \pm 0.1. $x_1: \pm$ 0.0003.				

DIBENZOTHIOPHENE	SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES
A.	<u>Saturated Hydrocarbons (including cycloalkanes)</u>
	cyclohexane decahydronaphthalene
в.	Alkenes
c.	Aromatic Hydrocarbons
	benzene
	1,2,3,4-tetrahydronaphthalene
D.	<u>Esters</u>
E.	Ethers
F.	Haloalkanes and Haloaromatic Hydrocarbons
G.	Alcohols
н.	Ketones
Ι.	Miscellaneous Pure Solvents
	pyridine
	thiophene

J. <u>Binary Solvent Mixtures</u>

-			1			
COMPONENTS:			ORIGINAL MEASUREMENTS:			
<pre>(1) Dibenzothiophene; C₁₂H₈S; [132-65-0] (2) Cyclohexane; C₆H₁₂; [110-82-7] VARIABLES:</pre>			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.			
			PREPARED F	BY:		
Temperature			W.E. Acree, Jr.			
EXPERIMENT	AL VALUES		<u>!</u>			
T/K	*2	×1	T/K	<i>x</i> 2	<i>x</i> 1	
320.6	0.9129	0.0871	343.0	0.6846	0.3154	
326.6	0.8871	0.1129	343.3	0.6654	0.3346	
328.2	0.8706	0.1294				
335.8	0.8001	0.1999				
		AUXILIARY	INFORMATION	м		
METHOD: AP	PARATUS/PROCEDU	RE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(1) 99 %, kee, from (2) Gold Compa	, Aldrich Che Wisconsin, U toluene. Label, 99.9+ any, was used	mical Company, Milwau- SA, was recrystallized %, Aldrich Chemical as received.	
noting th trace of	e temperature af solid solute dis	: which the last sappeared.	T/K: prec x ₁ : ± 0.0	ERRORS: cision <u>+</u> 0.1. 0003.		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 (1) Dibenzothiophene; C₁₂H₈S; [132-65-0] (2) Decahydronaphthalene; C₁₀H₁₈; [91-17-8] 	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E. Fluid Phase Equilibr. <u>1989</u> , 44, 305-345.		
VARIABLES:	PREPARED BI:		
Temperature	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
<i>T/K</i> x ₂ x ₁	τ/κ x ₂ x ₁		
311.3 0.8944 0.1056	333.9 0.7372 0.2628		
318.9 0.8607 0.1393			
325.8 0.8141 0.1859			
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	(1) 99.5 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from solution.		
in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.		
noting the temperature at which the last trace of solid solute disappeared.	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003.		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
 (1) Dibenzothiophene; C₁₂H, [132-65-0] (2) Benzene; C₆H₆; [71-43-1 	₈ s; 2]	Domanska, U.; Groves, F.R., Jr.; McLaughlin, E.		
		J. Chem. Eng. Data <u>1993</u> , 38, 88-94.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	×2	×1		
278.7	1.0000	0.0000		
278.0	0.9770	0.0230		
277.2	0.9570	0.0430		
276.6	0.9468	0.0532		
276.0	0.9402	0.0598		
278.2	0.9337	0.0663		
283.1	0.9216	0.0784		
285.7	0.9133	0.0867		
290.5	0.8990	0.1010		
294.7	0.8842	0.1152		
299.2	0.8670	0.1330		
301.3	0.8571	0.1429		
304.3	0.8427	0.1573		
306.7	0.8301	0.1699		
312.9	0.7934	0.2066		
319.2	0.7884	0.2516		
325.6	0.6962	0.3038		
330.7	0.6399	0.3601		
335.4	0.5869	0.4131		
340.8	0.5267	0.4733		
346.4	0.4649	0.5351		
350.3	0.4142	0.5858		
353.2	0.3577	0.6423		
372.0	0.0000	1.0000		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath thermometer.	and a precision	(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene.		
Mixtures of known concentring ass ampoules and place temperature to equilibrate were rotated while bath temperature	ations sealed ed in constant . Samples mperature slowly	(2) 99+ %, Aldrich Chemical Company, was fractionally distilled and stored over molecular sieves.		
increased. Solubility deter noting the temperature at a	which the last	ESTIMATED ERRORS:		
trace of solid solute disa	ppeared.	T/K: precision \pm 0.1. x_1 : \pm 0.0003.		

COMPONENTS:			ORIGINAL M	EASUREMENTS:	
<pre>(1) Dibenzothiophene; C₁₂H₈S; [132-65-0] (2) Benzene; C₆H₆; [71-43-2] VARIABLES:</pre>			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. <u>1988</u> , 16, 519-534.		
			PREPARED B	¥:	
Temperature			W.E. Acree	e, Jr.	
EXPERIMENTAL V	ALUES	<u></u>			· · · · · · · · · · · · · · · · · · ·
T/K	x ₂	x 1	T/K	*2	x 1
309.9	0.8104	0.1896	342.3	0.4856	0.5144
315.3	0.7754	0.2246			
327.8	0.6653	0.3347			
337.2	0.5638	0.4362			
		AUXILIARY	INFORMATION		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant			 (1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene. (2) Gold Label, 99.9+ %, Aldrich Chemical 		
were rotated	o equilibrate while bath te lubility det	Samples Imperature slowly ermined by	Compar	ny, was usea	as received.
noting the te	mperature at	which the last	ESTIMATED I	ERRORS:	
trace of soll	d solute disa	ippeared.	<i>T/K</i> : prec. <i>x</i> ₁ : <u>+</u> 0.00	ision <u>+</u> 0.1. 003.	

COMPONENTS:		ORIGINAL MEASUREMENTS:				
 Dibenzothiophene; C₁₂H₈S; [132-65-0] 1,2,3,4-Tetrahydronaphthalene; C₁₀H₁₂; [119-64-2] 			Coon, J.E. Fluid Pha	.; Auwaerter, se Equilibr.	, J.E.; McLaughlin, E. <u>1989</u> , 44, 305-345.	
VARIABLES:			PREPARED B	Y:		
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL V	ALUES					
T/K	x 2	×1	T/K	x 2	x 1	
308.7	0.7837	0.2163	337.8	0.5308	0.4692	
318.2	0.7219	0.2781				
326.6	0.6492	0.3508				
336.3	0.5534	0.4466				
	AUXILIARY INFORMATION					
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.			(1) 99.5 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- from solution.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.			
			ESTIMATED ERRORS:			
		T/K : precision \pm 0.1. x ₁ : \pm 0.0003.				

COMPONENTS:		ORIGINAL MEASUREMENTS:			
<pre>(1) Dibenzothiophene; C₁₂H₈S; [132-65-0] (2) Pyridine; C₅H₅N; [110-86-1]</pre>			Coon, J.E McLaughli J. Soluti	.; Sediawan, n, E. on Chem. <u>19</u>	W.B.; Auwaerter, J.E.; <u>88</u> , <i>16,</i> 519-534.
VARIABLES:		<u></u>	PREPARED B	Y:	
Temperature			W.E. Acree, Jr.		
EXPERIMENTAL V	ALUES				<u> </u>
T/K	*2	x 1	T/K	*2	x 1
306.5	0.7857	0.2143	334.7	0.5502	0.4498
313.0	0.7448	0.2552	335.2	0.5348	0.4652
322.8	0.6687	0.3313			
327.4	0.6216	0.3784		•	
		AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene. Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received. 		
			ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 0.0003.		

COMPONENTS:		ORIGINAL MEASUREMENTS:				
<pre>(1) Dibenzothiophene; C₁₂H₈S; [132-65-0] (2) Thiophene; C₄H₄S; [110-02-1] VARIABLES:</pre>			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.			
			J. Solution Chem. <u>1988</u> , 16, 519-534.			
			PREPARED BY:			
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL V	VALUES					_
T/K	<i>x</i> 2	×1	T/K	x2	×1	
309.3	0.7621	0.2379	328.1	0.6128	0.3872	
315.2	0.7224	0.2776	337.0	0.5050	0.4950	
322.7	0.6639	0.3361				
327.0	0.6257	0.3743				
		AUXILIARY	INFORMATION	4		
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.			(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			<pre>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</pre>			
noting the temperature at which the last trace of solid solute disappeared.			ESTIMATED	ERRORS:		
		$\begin{array}{c c} T/K: \text{ pred}\\ x_1: \pm 0.0 \end{array}$	cision <u>+</u> 0.1. 003.			

1,2-DIPHENYLBENZENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

cyclohexane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene

- D. <u>Esters</u>
- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons

tetrachloromethane

- G. <u>Alcohols</u>
- H. Ketones
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) 1,2-Diphenylbenzene; C ₁₈ H ₁₄ ;	McLaughlin, E.; Zainal, H.A.			
[84-15-1] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	J. Chem. Soc. <u>1960</u> , 3854-3857.			
VARIABLES:	PREPARED BY:			
Temperature	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
т/к ×2	x ₁			
296.0 0.6463	0.3537			
303.2 0.5004	0.4996			
313.6 0.2927	0.7073			
322.8 0.1045	0.8955			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	(1) Purity not given, Eastman Kodak, Roches- ter, New York, USA, was passed over an alumina column with light petroleum			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by	ether as eluant. (2) Purity, source, and purification method were not specified.			
noting the temperature at which the last trace of solid solute disappeared.	ESTIMATED ERRORS:			
	$T/K:$ precision \pm 0.1. $x_1: \pm$ 0.0003 (compiler).			

COMPONENTS:		ORIGINAL MEASUREMENTS:				
<pre>(1) 1,2-Diphenylbenzene; C (84-15-1)</pre>	18 ^H 14;	McLaughlin, E.; Zainal, H.A.				
(2) Benzene; C ₆ H ₆ ; [71-43-2	1	J. Chem. Soc. <u>1959</u> , 863-867.				
VARIABLES:	1	PREPARED BY:				
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
T/K	*2	* ₁				
301.2	0.4148	0.5852				
305.6	0.3558	0.6442				
318.0	0.1898	0.8102				
323.6	0.0987	0.9013				
AUXILIARY INFORMATION						
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath thermometer.	and a precision	(1) Purity not given, Eastman Kodak, Roches- ter, New York, USA, was passed over an alumina column with light petroleum				
Mixtures of known concentration glass ampoules and place temperature to equilibrate were rotated while bath temingreased. Solubility determines	ations sealed ed in constant . Samples mperature slowly rmined by	ether as eluant. (2) "AnalaR", was dried over sodium wire and freshly distilled before use.				
noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED ERRORS:				
		$T/K:$ precision \pm 0.1. $x_1: \pm 0.0003$ (compiler).				
COMPONENTS:			ORIGINAL MEASUREMENTS:			
--	-----------------	-----------	---	--	---	--
<pre>(1) 1,2-Diphenylbenzene; C₁₈H₁₄; [84-15-1] (2) Tetrachloromethane; CCl₄; [56-23-5]</pre>			McLaughlin, E.; Zainal, H.A. <i>J. Chem. So</i> c. <u>1960</u> , 2485-2488.			
VARIABLES:			PREPARED P	BY:		
Temperature			W.E. Acro	ee, Jr.		
EXPERIMENTA	L VALUES					
T/K	x2	×1	T/K	*2	×1	
302.0	0.4257	0.5743	323.0	0.1125	0.8875	
308.0	0.3293	0.6707				
314.8	0.2507	0.7493				
318.6	0.1814	0.8186				
		AUXILIARY	INFORMATION	4		
METHOD: APP	ARATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	IATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			(1) Purit ter, alum: ethe: (2) Anala driec and o ESTIMATED	ty not given, New York, US ina column wi r as eluant. aR grade, sou d over anhydr distilled bef ERRORS:	Eastman Kodak, Roches- SA, was passed over an th light petroleum urce not given, was cous calcium chloride fore use.	
			$\begin{array}{c} T/K: \text{ pred}\\ x_1: \pm 0.0 \end{array}$	cision <u>+</u> 0.1. 0003 (compile	r).	

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1,3-DIPHENYLBENZENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

cyclohexane

- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene

- D. <u>Esters</u>
- E. <u>Ethers</u>
- F. Haloalkanes and Haloaromatic Hydrocarbons

•

tetrachloromethane

- G. <u>Alcohols</u>
- H. Ketones
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

			OPTOTNAL N	CALID FUENTS .			
(1) 1,3-Diphenylbenzene; C ₁₈ H ₁₄ ;			ORIGINAL MEASUREMENTS:				
			McLaughli	.n, E.; Zaina	al, H.A.		
[92-06-8]] 2701 C H . 1	10-82-71	J. Chem.	Soc. 1960.	3854-3857		
(2) Cyclonexa	ine; c ₆ n ₁₂ ; [-	10-82-73	0. 01/6	<u> </u>	3034-3037.		
VARIABLES:			PREPARED P	IY:			
Temperature	Temperature			W.E. Acree, Jr.			
EXPERIMENTAL V	VALUES		. <u> </u>				
T/K	*2	×1	T/K	×2	<i>x</i> 1		
311.4	0.9230	0.0770	333.4	0.5925	0.4075		
320.6	0.8368	0.1632					
325.5	0.7579	0.2421					
329.9	0.6669	0.3331					
		AUXILIARY	INFORMATION	r			
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND) PURITY OF M	ATERIALS:		
Constant temp thermometer.	perature bath	and a precision	(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with light petroleum				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			ether as eluant.				
			(2) Purit	y, source an	d purification method		
			noca	pecified.			
noting the te	amperature at id solute dis	which the last appeared.	ESTIMATED	ERRORS:			
		-ppour out	T/K : precision \pm 0.1.				
			$ x_1: \pm 0.0$	003 (compile:	r).		

COMPONENTS: (1) 1,3-Diphenylbenzene; C ₁₈ H ₁₄ ; [92-06-8] (2) Benzene; C ₆ H ₆ ; [71-43-2]			ORIGINAL MEASUREMENTS: McLaughlin, E.; Zainal, H.A. J. Chem. Soc. <u>1959</u> , 863-867.			
Temperature			W.E. Acree, Jr.			
EXPER	IMENTAL V	ALUES				
	T/K	*2	x 1	T/K	*2	x ₁
	310.0	0.7173	0.2827	347.4	0.2429	0.7571
	320.2	0.6162	0.3838	350.8	0.1656	0.8344
	334.0	0.4534	0.5466			
	340.6	0.3593	0.6407			
			AUXILIARY	INFORMATIO	N	
METHOD: APPARATUS/PROCEDURE			SOURCE AN	D PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant			(1) Puri Unit alum ethe (2) "Ana	ty not given, ed Kingdom, w ina column wi r as eluant. laR", was dri	British Drug Houses, as passed over an th light petroleum ed over sodium wire	
temperature to equilibrate. Samples			and	freshly disti	lled before use.	

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

ESTIMATED ERRORS:

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

COMPON	NENTS:			ORIGINAL MEASUREMENTS:			
 (1) 1,3-Diphenylbenzene; C₁₈H₁₄; [92-06-8] (2) Tetrachloromethane; CCl₄; [56-23-5] 			McLaughlin, E.; Zainal, H.A. <i>J. Chem. Soc.</i> <u>1960</u> , 2485-2488.				
VARIA	BLES:			PREPARED BY	:		
Temperature			W.E. Acree	e, Jr.			
EXPERI	IMENTAL VAL	UES		•			
2	r/K	x2	x 1	T/K	x2	x 1	
3	312.6	0.7937	0.2063	343.2	0.5750	0.4250	
3	318.2	0.7391	0.2609				
3	328.6	0.6282	0.3718				
			AUXILIARY	INFORMATION			
METHO	D: APPARATU	IS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			 (1) Purity United alumin ether (2) AnalaR dried and di 	not given, Kingdom, wa a column wit as eluant. grade, sour over anhydro stilled befo	British Drug Houses, as passed over an ch light petroleum cce not given, was ous calcium chloride ore use.		
noting the temperature at which the last trace of solid solute disappeared.			ESTIMATED E $T/K:$ preci $x_1: \pm 0.00$	RRORS: .sion <u>+</u> 0.1. 03 (compiler	.).		

1,4-DIPHENYLBENZENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

- A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>
- B. <u>Alkenes</u>
- C. Aromatic Hydrocarbons

benzene

- D. <u>Esters</u>
- E. <u>Ethers</u>
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. <u>Alcohols</u>
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS :			ORIGINAL MEASUREMENTS:			
<pre>(1) 1,4-Diphenylbenzene; C₁₈H₁₄; [92-94-4] (2) Benzene; C₆H₆; [71-43-2]</pre>			McLaughlin, E.; Zainal, H.A. <i>J. Chem. Soc.</i> <u>1959</u> , 863-867.			
VARIABLES:			PREPARED F	BY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL VALUES			<u>l</u>		E	
T/K	x 2	<i>x</i> 1	T/K	*2	×1	
311.2	0.9929	0.0071	350.8	0.9721	0.0279	
333.4	0.9844	0.0156				
337.4	0.9822	0.0178				
341.2	0.9796	0.0204				
	_	AUXILIARY	INFORMATIO	N		
METHOD: APPARJ	TUS/PROCEDUR	E	SOURCE AN	D PURITY OF	MATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			(1) Puri Unit alum (2) "Ana and	ty not given ed Kingdom, ina column w llaR", was dr fresbly dist	, British Drug Houses, was passed over an ith benzene as eluant. ied over sodium wire illed before use.	
			ESTIMATED ERRORS:			
			$\frac{T/K: \text{ pre}}{x_1: \pm 0.}$	ecision <u>+</u> 0.1 0003 (compile	 er).	

SYSTEM INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

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