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SOLUBILITY DATA SERIES

Volume 59

POLYCYCLIC AROMATIC HYDROCARBONS: BINARY NON-AQUEOUS SYSTEMS

PART II: SOLUTES F–Z

SOLUBILITY DATA SERIES

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
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POLYCYCLIC AROMATIC HYDROCARBONS: BINARY NON-AQUEOUS SYSTEMS
PART II: SOLUTES F–Z

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CONTENTS

INTRODUCTION TO THE SOLUBILITY DATA SERIES

SOLUBILITY OF SOLIDS IN LIQUIDS

NATURE OF THE PROJECT

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

COMPILATIONS AND EVALUATIONS

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

Compilations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Evaluations

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

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

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

Critical Evaluation:

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

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

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

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

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

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

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

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

QUANTITIES AND UNITS USED IN COMPILATION AND EVALUATION OF SOLUBILITY DATA

Mixtures, Solutions and Solubilities

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

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

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

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

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

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

Physicochemical Quantities and Units

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$m_1 = n_1/n_2 M_2 \tag{9}$$

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

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

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

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

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

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:

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

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

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

$$\rho_1 = g_1/V = c_1M_1/V \tag{13}$$

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

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

$$r_{n,12} = n_1/n_2 \tag{14}$$

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

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

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

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

$$I_m = |z_+z_-|\nu m_i, \quad I_c = |z_+z_-|\nu c_i \tag{16}$$

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

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

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

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

12. *Density*, ρ:

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

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

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

Thermodynamics of Solubility

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

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

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

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

PREFACE

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

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

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

Polycyclic aromatic compounds are an important chemical class. They have been used as model compounds in coal liquefaction process design calculations, serve as the "parent" compound or base found in a number of drug molecules, and several are mutagens, carcinogens, or common organic pollutants resulting from oil spills. Moreover, many of the polycyclic aromatic compounds have very limited mole fraction solubilities, and from a thermodynamic modeling standpoint, saturated solutions are treated as infinitely dilute solutions. The solute is considered to be surrounded by solvent molecules and 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 measurements, as is the case with the majority of published solubility data for polycyclic aromatic compounds in binary solvent mixtures. Conventional methods of evaluation used in the *Solubility Data Series* are not applicable since data available from the different laboratories were not measured under the same conditions of temperature and solvent composition. For a more detailed treatment of solubility behavior, readers are referred to monographs by Acree (1), Grant and Higuchi (2), Hildebrand and Scott (3), James (4), Prausnitz *et al.* (5), and Shinoda (6).

BASIC THERMODYNAMIC PRINCIPLES

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

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

(3) mole fraction

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

or (4) volume fraction

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

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

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

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

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

where M_s is the molar mass of the solvent.

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

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

(a) The breaking of solute-solute interactions in the crystalline lattice;
(b) the breaking of solvent-solvent interactions, often referred to as cavity formation;
(c) the formation of solute-solvent interactions; and
(d) the 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 for solubility equilibrium of a component 1 in any system at temperature T, standard pressure p^o is:

$$\mu_1^*(\text{solid},T,p^o) = \mu_1(\text{sln},T,p^o) \qquad [6]$$

We choose the standard state for component 1 as the chemical potential of supercooled liquid 1 and T, p^o. Thus

$$\mu_1^*(\text{s},T,p^o) = \mu_1^o(\text{l},T,p^o) + \text{RT ln a}_1 \qquad [7]$$

from which the standard Gibbs energy of fusion is

$$\Delta_{\text{fus}}G_{\text{m}}^o/RT = -\ln \text{a}_1 \qquad [8]$$

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

$$\ln \text{a}_1(\text{s}) = \ln(\gamma_1 x_1) = -\Delta_{\text{fus}}H_{\text{m}}^o\ (T_{\text{m}} - T)/R\ T\ T_{\text{m}} + \Delta C_{\text{p}}\ (T_{\text{m}} - T)/RT$$
$$- (\Delta C_{\text{p}}/R)\ \ln(T_{\text{m}}/T) \qquad [9]$$

for the solubility of a crystalline solute in a liquid solvent, where $\Delta_{\text{fus}}H_{\text{m}}^o$ is the standard enthalpy of fusion. In the above expression γ_1 is the activity coefficient of the solute. The expression for $\text{a}_1(\text{s})$ must include additional term(s) if the solid undergoes a phase transition (7,8).

MELTING TEMPERATURES AND ENTROPIES OF FUSION

Melting point temperatures and enthalpy of fusion data are tabulated in Table I for 29 polycyclic aromatic hydrocarbons and hetero-atom derivatives. Except where noted, numerical values were taken from published compilations (9,10). For molecules not listed in the table it is possible to estimate $\Delta_{\text{fus}}H_{\text{m}}^o$ 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 mass centers in the crystal to the more randomized, expanded

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

Polycyclic Aromatic Compound	T_m/K	$\Delta_{fus}H_m^{\circ}$/kJ mol^{-1}	$\Delta_{fus}S_m^{\circ}$/J mol^{-1} K^{-1}
Naphthalene	351.3	19.12	54.4
Acenaphthylene	362.1	10.96	30.3
Dibenzofuran	355.7	18.60	52.3
Dibenzothiophene	371.0	15.30	41.2
Thianthrene	428.5	25.44	59.4
Carbazole	516.2	29.42	57.0
Acenaphthene	366.6	21.54	58.8
Acridine	452.4	19.70	43.5
Fluorene	388.0	19.58	50.5
Xanthene	373.7	19.20	51.4
Anthracene	492.7	28.83	58.5
Phenanthrene	372.4	16,47	44.2
Pyrene	424.4	17.11	40.3
Fluoranthene	381.0	18.87	49.5
Chrysene	531.4	26.15	49.2
Triphenylene	473.5	25.10	53.0
Benz[a]anthracene	434.3	21.38	49.2
Benzo[c]phenanthrene	334.7	16.31	48.7
Perylene	553.9	31.75	57.3
Benzo[a]pyrene	454.2	17.32	38.1
Benzo[ghi]perylene	554.2	17.37	31.3
Dibenz[a,c]anthracene	553.5	25.82	46.6
Dibenz[a,h]anthracene	544.2	31.16	57.3
Benzo[rst]pentaphene	556.8	27.87	50.1
Dibenzo[def,p]chrysene	501.2	24.68	49.2
Dibenzo[a,e]pyrene	520.2	30.50	58.6
Phthalazine	364.5	13.32	36.5
Quinazoline	320.9	16.95	52.8
Quinoxaline	305.7	11.80	38.6

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[a] Melting temperatures, T_m, 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 (25).

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, $\Delta_{fus}S_m^o$, is equal to the entropy of the liquid state minus the entropy of the crystal:

$$\Delta_{fus}S_m^o = -R \ln P_{fus} \qquad [10]$$

where P_{fus} is the ratio of the number of molecular arrangements of molecules in the crystal to the number of molecular arrangements of molecules in 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 always independent (*i.e.*, $P_{fus} = P_{trans}\, P_{rot}$), then entropies must be additive

$$\Delta_{fus}S_m^o = \Delta_{trans}S_m^o + \Delta_{rot}S_m^o \qquad [11]$$

The appearance of translational entropy of fusion can be visualized by a two-dimensional analogy involving a field of checkers or disks that has been trapped into a nearly close-packed two-dimensional crystalline arrangement. When the crystal melts, a slight expansion and randomization of the disk positions occur. The probability of two-dimensional fusion is equal to the total number of arrangements of the disks that are possible within the area allotted for the solid divided by the corresponding number of arrangements that are possible within the area allotted to the liquid melt. This, in turn, is related to the ratio of the free areas available within each phase for the disks. 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 $\Delta_{trans}S_m^o = 14.6$ J mol^{-1} K^{-1} for the translational melting contribution to the entropy of fusion, though the authors did state that nonspherical molecules generally have a somewhat larger volume change associated with melting.

The rotational entropy of fusion results from differences in rotational degrees of freedom. In the crystal, molecules (with their centers of mass fixed) can wobble or vibrate approximately 10° in the spherical coordinates ϕ and θ from their most stable position after averaging over all axes. Molecules in the liquid phase have much greater orientational freedom and can rotate over a much wider range of ϕ and θ. If it is assumed for simplicity that liquid molecules can rotate freely, then any reference point will trace out a sphere about the center of gravity of the molecule. The reference point traces out only a spherical segment if the molecule's motion is restricted, as would be the case for the crystalline lattice. A ± 10° variation in ϕ and θ corresponds to a spherical segment that is roughly 0.00754 times that of a sphere of the same radius, or roughly a rotational entropy of fusion of $\Delta_{fus}S_m^o = 41.8$ J mol^{-1}

K^{-1}. On the basis of the above discussion (11), the total entropy of fusion for a rigid polycyclic aromatic compound would be $\Delta_{fus}S_m^o = \Delta_{trans}S_m^o + \Delta_{rot}S_m^o \approx 56.4$ J mol^{-1} K^{-1}, which is in reasonable (though by no means perfect) agreement with experimental values listed in Table I.

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

For acyclic and aromatic hydrocarbons

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

For cyclic hydrocarbons

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

For polycyclic molecules

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

where $K = \Sigma\, n_k$, n refers to the number of equivalent methylene groups necessary to simulate the size of the ring, R is the total number of ring atoms and N is 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 estimation 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 multiplying $\Delta_{fus}S_m^o$ by the observed melting point temperature, T_m. 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 $\Delta_{fus}S_m^o$ and $\Delta_{fus}H_m^o$. Average difference between predicted and observed values was approximately 7 %.

SOLUBILITIES IN SINGLE SOLVENTS

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

(a) For a given solid-solvent system, the solubility increases with increasing temperature. The rate of increase is approximately proportional to the enthalpy of fusion and, to a first approximation, does not depend upon the melting 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 solubilities of small solute molecules.. This is not too surprising because the Flory-Huggins model

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

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

provides a more realistic description of solution ideality in polymer solutions. The corresponding expression for solubility (as a volume fraction eqn. [3]) is given by

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

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

SCATCHARD-HILDEBRAND SOLUBILITY PARAMETER THEORY

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

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

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

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

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

SOLUBILITIES IN BINARY SOLVENT MIXTURES

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

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

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

TABLE II. Comparison Between Experimental and Predicted Naphthalene Solubilities

Solvent	δ_2[a]	$V_{m,2}/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	x_1(exp)[b]	x_1(calc)
Dichloromethane	20.21	64.50	0.330	0.311
Chlorobenzene	19.78	102.26	0.311	0.312
Benzene	18.74	89.41	0.292	0.305
Trichloromethane	18.74	80.64	0.339	0.305
Methylbenzene	18.27	106.84	0.292	0.295
Ethylbenzene	18.08	123.08	0.289	0.289
Tetrachloromethane	17.49	97.08	0.255	0.275
Cyclohexane	16.75	108.76	0.147	0.242
Methylcyclohexane	15.95	128.32	0.147	0.189
n-Octane	15.42	163.48	0.142	0.146
n-Heptane	15.34	147.48	0.130	0.144
n-Hexane	14.87	131.51	0.122	0.119
Carbon disulfide	20.29	60.62	0.283	0.311

[a] $\delta_2/\mathrm{J}^{1/2}\ \mathrm{cm}^{-3/2}$.

[b] Experimental solubilites were determined by Chang (26).

TABLE III. Comparison Between Experimental and Predicted Biphenyl Solubilities

Solvent	δ_2[a]	$V_{m,2}/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	x_1(exp)[b]	x_1(calc)
Dichloromethane	20.21	64.50	0.412	0.384
Chlorobenzene	19.78	102.26	0.397	0.384
Benzene	18.74	89.41	0.381	0.374
Trichloromethane	18.74	80.64	0.422	0.375
Methylbenzene	18.27	106.84	0.377	0.362
Ethylbenzene	18.08	123.08	0.363	0.353
Tetrachloromethane	17.49	97.08	0.342	0.340
Cyclohexane	16.75	108.76	0.190	0.295
Methylcyclohexane	15.95	128.32	0.183	0.215
n-Octane	15.42	163.48	0.147	0.147
n-Heptane	15.34	147.48	0.138	0.145
n-Hexane	14.87	131.51	0.124	0.112
Carbon disulfide	20.29	60.62	0.369	0.384

[a] $\delta_2/\mathrm{J}^{1/2}\ \mathrm{cm}^{-3/2}$.

[b] Experimental solubilities were determined by Chang (26).

of the pure components. Whereas this particular application of the solubility parameter theory has certain practical advantages in that it requires only a minimal number of experimental observations, a more flexible expression for binary solvent systems can be derived by replacing the individual δ_i values with the measured solubilities in the pure solvents and the measured thermodynamic excess properties of the solvent mixture.

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

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

and multiply out the squared term

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

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

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

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

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

in terms of solubility parameters.

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

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

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.

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

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

derived by Martin and co-workers (19-21) reproduces very accurately the solubility behavior of many crystalline nonelectrolytes in very nonideal binary solvent mixtures. Numerical values of the various A_i-coefficients are computed from the solubility data using a least squares analysis, provided that the solubility parameters of all solvent components are known. 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.

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

$$(Z^E{}_{123})_{exp} - (Z^E{}_{123})_{calc} = x_1\ x_2\ x_3\ Q_{123} \qquad [26]$$

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

$$Q_{123} = A_{123} + \Sigma\ B_{12}{}^{(i)}\ (x_1 - x_2)^i + \Sigma\ B_{13}{}^{(j)}\ (x_1 - x_3)^j + \Sigma\ B_{23}{}^{(k)}\ (x_2 - x_3)^k \qquad [27]$$

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 data base for solid solute solubilities 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:

$$\ln x_1 = x_2{}^{(s)} \ln (x_1)_2 + x_3{}^{(s)} \ln (x_1)_3 + x_2{}^{(s)}\ x_3{}^{(s)}\ \Sigma\ S_i\ (x_2{}^{(s)} - x_3{}^{(s)})^i \qquad [28]$$

or Modified Wilson equation

$$\begin{aligned}\ln (a_1(s)/x_1) = 1 &- x_2{}^{(s)}\ \{1 - \ln [a_1(s)/(x_1)_2]\}/(x_2{}^{(s)} + x_3{}^{(s)}\ \Lambda_{23}{}^{adj}) \\ &- x_3{}^{(s)}\ \{1 - \ln [a_1(s)/(x_1)_3]\}/(x_2{}^{(s)}\ \Lambda_{32}{}^{adj} + x_3{}^{(s)}) \qquad [29]\end{aligned}$$

where the various S_i and $\Lambda_{ij}{}^{adj}$ "curve-fit" parameters can be evaluated via least squares analysis. A summarized comparison presenting the descriptive abilities of eqns. [29] and [28] is summarized in Tables IV and V, respectively. For pyrene, a value of $a_1(s)$ = 0.1312 was used in all Modified Wilson computations. The actual solubilities are

TABLE IV. Mathematical Representation of Pyrene Solubilities in Select Binary Mixtures using the Modified Wilson Equation

Solvent (2) + Solvent (3)	$\Lambda_{ij}^{adj,a}$	% Dev.[b]
n-Hexane + 1-propanol	1.340 1.348	1.4
n-Heptane + 1-propanol	1.249 1.577	0.7
n-Octane + 1-propanol	1.032 1.936	1.1
Cyclohexane + 1-propanol	1.749 1.281	0.6
Methylcyclohexane + 1-propanol	1.605 1.450	0.4
2,2,4-Trimethylpentane + 1-propanol	0.804 1.744	0.6
n-Hexane + 2-propanol	1.080 1.628	0.4
n-Heptane + 2-propanol	1.072 1.908	0.9
n-Octane + 2-propanol	0.936 2.248	1.1
Cyclohexane + 2-propanol	1.464 1.556	0.8
Methylcyclohexane + 2-propanol	1.404 1.744	1.0
2,2,4-Trimethylpentane + 2-propanol	0.904 1.752	0.8

---

[a] Adjustable parameters for the Modified Wilson equation are ordered as Λ_{23}^{adj} and then Λ_{32}^{adj}. See eqn. [29] in text.

[b] % Dev. $= (100/N)\ \Sigma\ |\ \ln\ [x_A(cal)/x_A(exp)]\ |$.

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

Solvent (2) + Solvent (3)	S_i[a]	% Dev[b]	S_i[a]	% Dev[b]
n-Hexane + 1-propanol	1.334 - 0.045	2.3	1.188 0.073 0.544	0.6
n-Heptane + 1-propanol	1.476 - 0.190	1.1	1.383 - 0.202 0.280	0.4
n-Octane + 1-propanol	1.703 - 0.627	2.4	1.528 - 0.419 0.701	0.3
Cyclohexane + 1-propanol	1.459 0.232	0.9	1.396 0.268 0.226	0.7
Methylcyclohexane + 1-propanol	1.544 - 0.042	0.8	1.507 - 0.011 0.138	0.4
2,2,4-Trimethylpentane + 1-propanol	0.936 - 0.352	0.9	0.864 - 0.255 0.304	0.1
n-Hexane + 2-propanol	1.511 - 0.302	0.7	1.460 - 0.265 0.190	0.3
n-Heptane + 2-propanol	1.948 - 0.636	2.0	1.799 - 0.478 0.581	0.2
n-Octane + 2-propanol	2.225 - 1.082	3.0	1.988 - 0.795 0.942	0.4
Cyclohexane + 2-propanol	1.830 - 0.219	1.4	1.726 - 0.165 0.372	0.1
Methylcyclohexane + 2-propanol	2.054 - 0.380	1.8	1.921 - 0.279 0.491	0.3
2,2,4-Trimethylpentane + 2-propanol	1.423 - 0.345	1.4	1.329 - 0.232 0.378	0.5

---

[a] Regressional coefficients in the Combined NIBS/Redlich-Kister mathematical representation. Coefficients are ordered as S_0, S_1 and S_2. First and third columns refer to the best two- and three-parameter equation, respectively. See eqn. [28] of text.

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

given in the data compilation portion of this volume. Careful examination of Tables IV and V reveals that both equations provide a reasonable mathematical representation of the anthracene solubility data in all systems considered. Back-calculated and observed values generally differ by less than ± 1.5 %, 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 ± 3 %. 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.

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FLUORANTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,2,4,5-tetramethylbenzene
naphthalene
2-methylnaphthalene
2,7-dimethylnaphthalene
fluorene
anthracene
phenanthrene
acenaphthene
chrysene

D. Esters

E. Ethers

1,4-dioxane

F. Haloalkanes and Haloaromatic Hydrocarbons

tetrachloromethane
chlorobenzene

G. Alcohols

methanol
ethanol
1-octanol
1-hydroxy-2-methylbenzene

H. Ketones

2-propanone

I. Miscellaneous Pure Solvents

pyridine
nitrobenzene
dimethyl sulfoxide
1,3-dinitrobenzene
1,4-dinitrobenzene
1,3,5-trinitrobenzene
1,2,3,5-tetranitrobenzene
2,4-dinitromethylbenzene
2,4-dinitrophenol
2,4,6-trinitromethylbenzene
2,4,6-trinitromethoxybenzene

2,4,6-trinitroaniline
2-chloro-1,3,5-trinitrobenzene
3-methyl-2,4,6-trinitrophenol

J. Binary Solvent Mixtures

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.8	0.9796	0.0204	344.2	0.8237	0.1763
317.6	0.9600	0.0400			
325.5	0.9401	0.0599			
338.2	0.8809	0.1191			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
318.0	0.7826	0.2174
329.2	0.6989	0.3011
337.6	0.6174	0.3826
350.4	0.4669	0.5331

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Benzene; C_6H_6; [71-43-2]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
278.7	1.000	0.000	(2)
276.5	0.979	0.021	(2)
274.9	0.956	0.044	(2)
274.4	0.943	0.057	Eutectic
277.2	0.935	0.065	(1)
280.9	0.924	0.076	(1)
290.2	0.898	0.102	(1)
295.5	0.877	0.123	(1)
300.8	0.856	0.144	(1)
307.7	0.829	0.171	(1)
309.5	0.813	0.187	(1)
315.8	0.780	0.220	(1)
324.4	0.714	0.286	(1)
333.2	0.651	0.349	(1)
343.3	0.569	0.431	(1)
348.3	0.511	0.489	(1)
383.2	0.000	1.000	(1)

Authors report the eutectic point occurs at x_1 = 0.057 and T/K = 274.4.

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.* 1939, *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 distilled before use.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Methylbenzene; C_7H_8; [108-88-3]	**ORIGINAL MEASUREMENTS:** Krezewki, R.; Smutek, M. *Collection Czech. Chem. Commun.* 1967, *32*, 1258-1259.
VARIABLES: T/K = 293	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.895	0.105

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.
(2) 99 %, Urxovy Zavody, Czech., was used as received.

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
352.4	1.000	0.000	(2)
347.4	0.915	0.085	(2)
343.3	0.840	0.160	(2)
339.4	0.762	0.238	(2)
336.5	0.715	0.285	(2)
332.7	0.650	0.350	(2)
332.2	0.618	0.382	Eutectic
334.5	0.601	0.399	(1)
340.4	0.552	0.448	(1)
349.2	0.462	0.538	(1)
358.2	0.351	0.649	(1)
368.2	0.218	0.782	(1)
374.8	0.118	0.882	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.382 and T/K = 332.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Naphthalene; $C_{10}H_8$; [91-20-3]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
353.4	1.000	0.000	(2)
346.3	0.883	0.117	(2)
338.5	0.753	0.247	(2)
332.2	0.663	0.337	(2)
329.0	0.610	0.390	Eutectic
330.9	0.589	0.411	(1)
337.1	0.539	0.461	(1)
343.5	0.471	0.519	(1)
352.8	0.386	0.614	(1)
361.4	0.293	0.707	(1)
374.2	0.125	0.875	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.390 and T/K = 329.0.

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.* 1939, *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) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
307.3	1.000	0.000	(2)
298.4	0.899	0.101	(2)
296.5	0.871	0.129	(2)
293.8	0.835	0.165	(2)
292.5	0.799	0.201	Eutectic
297.9	0.764	0.236	(1)
310.2	0.711	0.289	(1)
317.4	0.662	0.338	(1)
330.3	0.586	0.414	(1)
341.3	0.508	0.492	(1)
349.7	0.420	0.580	(1)
356.6	0.344	0.656	(1)
365.1	0.242	0.758	(1)
375.6	0.102	0.898	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.201 and T/K = 292.5.

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.* 1939, *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: (1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,7-Dimethylnaphthalene; $C_{12}H_{12}$; [582-16-1]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
370.2	1.000	0.000	(2)
365.3	0.916	0.084	(2)
358.1	0.792	0.208	(2)
352.6	0.704	0.296	(2)
344.2	0.572	0.428	(2)
339.2	0.518	0.482	Eutectic
340.7	0.491	0.509	(1)
349.3	0.407	0.593	(1)
356.4	0.328	0.672	(1)
363.8	0.242	0.758	(1)
372.6	0.136	0.864	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.482 and T/K = 339.2.

AUXILIARY INFORMATION

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

COMPONENTS:

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

(2) Fluorene; $C_{13}H_{10}$; [86-73-7]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
387.2	1.000	0.000	(2)
380.7	0.901	0.099	(2)
373.2	0.805	0.195	(2)
363.7	0.702	0.298	(2)
353.8	0.611	0.389	(2)
345.3	0.523	0.477	(2)
342.2	0.481	0.519	Eutectic
343.1	0.470	0.530	(1)
347.9	0.429	0.571	(1)
352.6	0.375	0.625	(1)
360.0	0.296	0.704	(1)
368.1	0.203	0.797	(1)
376.3	0.095	0.905	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at $x_1 = 0.519$ and $T/K = 342.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
489.7	1.000	0.000	(2)
475.1	0.822	0.178	(2)
467.4	0.731	0.269	(2)
459.7	0.645	0.355	(2)
449.4	0.544	0.456	(2)
435.2	0.434	0.566	(2)
419.9	0.329	0.671	(2)
395.7	0.196	0.804	(2)
387.3	0.170	0.830	(2)
380.2	0.141	0.859	(2)
374.2	0.140	0.860	(2)
375.0	0.116	0.884	(1)
376.5	0.094	0.906	(1)
377.8	0.070	0.930	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.870 and T/K = 374.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Phenanthrene; $C_{14}H_{10}$; [85-01-8]	Kravchenko, V.M.; Pastukhova, I.S. *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	x_2	x_1	Solid Phase
372.5	1.000	0.000	(2)
368.7	0.935	0.065	(2)
363.8	0.844	0.156	(2)
355.3	0.706	0.294	(2)
349.6	0.609	0.391	(2)
346.2	0.540	0.460	Eutectic
347.5	0.520	0.480	(1)
353.4	0.437	0.563	(1)
358.5	0.356	0.644	(1)
365.0	0.262	0.738	(1)
375.7	0.104	0.896	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.460 and T/K = 346.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
368.3	1.000	0.000	(2)
362.3	0.908	0.092	(2)
358.1	0.837	0.163	(2)
348.2	0.707	0.293	(2)
339.4	0.612	0.388	(2)
335.3	0.571	0.429	(2)
335.0	0.562	0.438	Eutectic
340.8	0.508	0.492	(1)
350.7	0.394	0.606	(1)
363.4	0.248	0.752	(1)
368.8	0.185	0.815	(1)
383.2	0.000	1.000	(1)

Authors report eutectic point occurs at x_1 = 0.438 and T/K = 335.0.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Chrysene; $C_{18}H_{12}$; [218-01-9]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
528.2	1.000	0.000	(2)
519.2	0.910	0.090	(2)
510.5	0.805	0.195	(2)
498.4	0.707	0.293	(2)
486.2	0.596	0.404	(2)
474.5	0.502	0.498	(2)
457.2	0.398	0.602	(2)
442.4	0.309	0.691	(2)
418.8	0.201	0.799	(2)
403.2	0.154	0.846	(2)
387.3	0.103	0.897	(2)
378.2	0.082	0.918	(2)
378.7	0.061	0.939	(1)
383.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	1.54

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.

c_1: ± 5% (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.0	0.8968	0.1032	333.6	0.7016	0.2984
313.4	0.8576	0.1424			
320.2	0.8179	0.1821			
326.2	0.7722	0.2278			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003 (compiler).

COMPONENTS:

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

(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

$T/K = 296$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
23.0	1.61

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

$T/K = 296$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
23.0	0.0704

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Ethanol; C_2H_6O; [64-17-5]	Krezewki, R.; Smutek, M. *Collection Czech. Chem. Commun.* 1967, *32*, 1258-1259.
VARIABLES:	**PREPARED BY:**
T/K = 293	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.9949	0.00514

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.
(2) Commercial sample, purity and source not given, was dehydrated and distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D. *Environ. Sci. Technol.* 1985, *19*, 522-529.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.1726

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639-646.
VARIABLES:	**PREPARED BY:**
T/K = 296	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.198

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Hydroxy-2-methylbenzene; C_7H_8O; [95-48-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639-646.
VARIABLES:	**PREPARED BY:**
T/K = 296	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.0534

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.9289	0.0711

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.
(2) Commercial sample, purity and source not given, was dehydrated and distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.842	0.158

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, coal tar extract, was recrystallized several times from ethanol to give a melting point temperature of 110.0-110.3 °C.
(2) Purity not given, Urxovy Zavody, Czech., treated with potassium permanganate, dried over potassium hydroxide and then distilled before use.

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	1.98

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.

c_1: ± 5% (relative error; compiler).

COMPONENTS:

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

(2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	1.09

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.

c_1: ± 5% (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
363.2	1.000	0.000	(2)
356.2	0.879	0.121	(2)
350.2	0.784	0.216	(2)
346.2	0.752	0.248	(2)
342.2	0.740	0.260	(2)
344.7	0.730	0.270	(2)
342.2	0.690	0.310	1:1 Compound
347.2	0.655	0.345	1:1 Compound
348.0	0.633	0.367	1:1 Compound
349.2	0.601	0.399	1:1 Compound
349.7	0.568	0.432	1:1 Compound
349.7	0.522	0.478	1:1 Compound
350.2	0.502	0.498	1;1 Compound
349.2	0.430	0.570	(2)
349.2	0.385	0.615	(2)
352.7	0.307	0.693	(2)
382.7	0.000	1.000	(2)

Author reports formation of a 1:1 fluoranthene - 1,3-dinitrobenzene light yellow molecular compound having a melting point temperature of 350.2 K. Two eutectic points occur at x_1 = 0.290 and T/K = 341.2, and at x_1 = 0.560 and T/K = 344.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,4-Dinitrobenzene; $C_6H_4N_2O_4$; [100-25-4]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
446.7	1.000	0.000	(2)
426.2	0.706	0.294	(2)
411.2	0.568	0.432	(2)
388.2	0.406	0.594	(2)
370.2	0.323	0.667	(2)
363.2	0.231	0.769	(1)
370.2	0.166	0.834	(1)
379.2	0.056	0.944	(1)
382.7	0.000	1.000	(1)

Author reports that a single eutectic point occurs at x_1 = 0.701 and T/K = 353.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,3,5-Trinitrobenzene; $C_6H_3N_3O_6$; [99-35-4]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
396.2	1.000	0.000	(2)
413.0	0.893	0.107	1:1 Compound
437.7	0.828	0.172	1:1 Compound
461.7	0.738	0.262	1:1 Compound
461.5	0.714	0.286	1:1 Compound
476.2	0.581	0.419	1:1 Compound
477.7	0.489	0.511	1:1 Compound
477.2	0.469	0.531	1:1 Compound
473.2	0.376	0.624	1:1 Compound
456.2	0.283	0.717	1:1 Compound
397.7	0.161	0.839	1:1 Compound
379.2	0.049	0.951	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 1,3,5-trinitrobenzene yellow molecular compound having a melting point temperature of 478.2 K. Two eutectic points occur at x_1 = 0.040 and T/K = 376.2, and at x_1 = 0.868 and T/K = 371.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,2,3,5-Tetranitrobenzene; $C_6H_2N_4O_8$; [3698-53-1]	**ORIGINAL MEASUREMENTS:** Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
399.2	1.000	0.000	(2)
385.2	0.939	0.061	(2)
389.2	0.836	0.164	(2)
393.2	0.680	0.320	1:1 Compound
393.2	0.672	0.328	1:1 Compound
405.2	0.561	0.439	1:1 Compound
405.2	0.522	0.478	1:1 Compound
407.2	0.501	0.499	1:1 Compound
403.2	0.402	0.598	1:1 Compound
397.2	0.360	0.640	1:1 Compound
383.2	0.284	0.716	1:1 Compound
370.2	0.217	0.783	1:1 Compound
361.2	0.202	0.798	1:1 Compound
367.2	0.142	0.858	(1)
371.2	0.127	0.873	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 1,2,3,5-tetranitrobenzene brown molecular compound having a melting point temperature of 407.2 K. Two eutectic points occur at x_1 = 0.253 and *T*/K = 383.2, and at x_1 = 0.801 and *T*/K = 357.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details given in paper.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS: *T*/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,4-Dinitromethylbenzene; $C_7H_6N_2O_4$; [121-14-2]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
344.2	1.000	0.000	(2)
341.2	0.941	0.059	(2)
336.2	0.853	0.147	(2)
332.2	0.770	0.230	1:1 Compound
334.2	0.747	0.253	1:1 Compound
338.7	0.695	0.305	1:1 Compound
342.7	0.636	0.364	1:1 Compound
346.7	0.552	0.448	1:1 Compound
347.7	0.543	0.457	1:1 Compound
348.7	0.452	0.548	1:1 Compound
347.2	0.402	0.598	1:1 Compound
347.7	0.221	0.779	(1)
363.2	0.198	0.802	(1)
375.7	0.090	0.910	(1)
382.7	0.000	1.000	(1)

- Author reports formation of a 1:1 fluoranthene - 2,4-dinitromethylbenzene yellow molecular compound having a melting point temperature of 348.7 K. Two eutectic points occur at $x_1 = 0.224$ and T/K = 330.2, and at $x_1 = 0.640$ and T/K = 341.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,4-Dinitrophenol; $C_6H_4N_2O_5$; [51-28-5]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
386.7	1.000	0.000	(2)
379.2	0.874	0.126	(2)
375.0	0.790	0.210	(2)
367.2	0.695	0.305	(2)
360.2	0.622	0.378	1:1 Compound
360.7	0.600	0.400	1:1 Compound
364.2	0.505	0.495	1:1 Compound
365.2	0.491	0.509	1:1 Compound
361.2	0.395	0.605	1:1 Compound
351.4	0.303	0.697	(1)
356.2	0.276	0.724	(1)
356.2	0.275	0.725	(1)
372.2	0.155	0.845	(1)
378.2	0.053	0.947	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 2,4-dinitrophenol yellow molecular compound having a melting point temperature of 365.2 K. Two eutectic points occur at $x_1 = 0.388$ and $T/K = 358.2$, and at $x_1 = 0.688$ and $T/K = 348.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,4,6-Trinitromethylbenzene; $C_7H_5N_3O_6$; [118-96-7]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
354.7	1.000	0.000	(2)
368.2	0.792	0.208	1:1 Compound
387.2	0.708	0.292	1:1 Compound
399.2	0.639	0.361	1:1 Compound
405.2	0.567	0.433	1:1 Compound
404.7	0.443	0.557	1:1 Compound
405.2	0.436	0.564	1:1 Compound
386.2	0.285	0.715	1:1 Compound
380.2	0.263	0.737	1:1 Compound
363.2	0.212	0.788	Eutectic
373.4	0.138	0.862	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 2,4,6-trinitromethylbenzene yellow compound having a melting point temperature of 406.2 K. Two eutectic points occur at x_1 = 0.150 and T/K = 345.7, and at x_1 = 0.788 and T/K = 362.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,4,6-Trinitromethoxybenzene; $C_7H_5N_3O_7$; [606-35-9]	**ORIGINAL MEASUREMENTS:** Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
341.2	1.000	0.000	(2)
338.2	0.928	0.072	(2)
334.7	0.865	0.135	(2)
332.2	0.792	0.208	1:1 Compound
337.7	0.755	0.245	1:1 Compound
344.7	0.647	0.353	1:1 Compound
346.0	0.627	0.372	1:1 Compound
347.2	0.537	0.463	1:1 Compound
348.2	0.512	0.488	1:1 Compound
347.2	0.454	0.546	1:1 Compound
348.2	0.338	0.662	(1)
359.7	0.280	0.720	(1)
374.7	0.127	0.873	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 2,4,6-trinitromethoxybenzene yellow molecular compound having a melting point temperature of 348.2 K. Two eutectic points occur at x_1 = 0.185 and T/K = 328.2, and at x_1 = 0.630 and T/K = 341.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE: No experimental details given in paper.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 2,4,6-Trinitroaniline; $C_6H_4N_4O_6$; [489-98-5]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

J. Chem. Soc. Japan 1940, *15*, 259-270.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
461.7	1.000	0.000	(2)
444.7	0.777	0.223	(2)
453.7	0.648	0.352	1:1 Compound
464.2	0.515	0.485	1:1 Compound
464.2	0.482	0.518	1:1 Compound
460.7	0.384	0.616	1:1 Compound
459.2	0.352	0.648	1:1 Compound
441.2	0.262	0.738	1:1 Compound
414.2	0.158	0.842	1:1 Compound
390.7	0.099	0.901	1:1 Compound
378.2	0.053	0.947	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 2,4,6-trinitroaniline brownish-yellow compound having a melting point temperature of 464.7 K. Two eutectic points occur at x_1 = 0.267 and T/K = 439.2, and at x_1 = 0.928 and T/K = 375.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 2-Chloro-1,3,5-trinitrobenzene; $C_6H_2ClN_3O_6$; [88-88-0]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

J. Chem. Soc. Japan 1940, *15*, 259-270.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
356.2	1.000	0.000	(2)
346.7	0.827	0.173	1:1 Compound
370.2	0.739	0.261	1:1 Compound
384.2	0.636	0.364	1:1 Compound
390.2	0.574	0.426	1:1 Compound
392.2	0.464	0.536	1:1 Compound
392.2	0.460	0.540	1:1 Compound
385.2	0.375	0.625	1:1 Compound
379.2	0.330	0.670	1:1 Compound
371.2	0.154	0.846	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 2-chloro-1,3,5-trinitrobenzene orangish-yellow compound with melting point of 393.2 K. Two eutectic points occur at x_1 = 0.156 and T/K = 340.2, and at x_1 = 0.738 and T/K = 353.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 3-Methyl-2,4,6-trinitrophenol; $C_7H_5N_3O_7$; [602-99-3]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

J. Chem. Soc. Japan 1940, *15*, 259-270.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
381.7	1.000	0.000	(2)
383.2	0.890	0.110	1:1 Compound
412.2	0.677	0.323	1:1 Compound
416.2	0.569	0.431	1:1 Compound
417.2	0.483	0.517	1:1 Compound
416.2	0.432	0.568	1:1 Compound
412.2	0.364	0.636	1:1 Compound
399.7	0.214	0.786	1:1 Compound
385.2	0.138	0.862	1:1 Compound
378.2	0.117	0.883	1:1 Compound
381.0	0.038	0.962	(1)
382.7	0.000	1.000	(1)

Author reports formation of a 1:1 fluoranthene - 3-methyl-2,4,6-trinitrophenol yellow compound having a melting point of 417.2 K. Two eutectic points occur at x_1 = 0.082 and T/K = 374.2, and at x_1 = 0.890 and T/K = 374.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

FLUORENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,2,3,4-tetrahydronaphthalene
ethylbenzene
1,3-dimethylbenzene
1,4-dimethylbenzene
1,2,4,5-tetramethylbenzene
naphthalene
2-methylnaphthalene
2,7-dimethylnaphthalene
fluoranthene
acenaphthene
chrysene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

tetrachloromethane
chlorobenzene

G. Alcohols

methanol
ethanol
1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

nitrobenzene
pyridine
aniline
thiophene
1,2-dinitrobenzene
1,3-dinitrobenzene
1,4-dinitrobenzene
1,3,5-trinitrobenzene
1,2,3,5-tetranitrobenzene
2,4-dinitromethylbenzene
2,4,6-trinitromethylbenzene
2,4-dinitrophenol

2,4,6-trinitrophenol
6-methyl-2,3,4-trinitrophenol

J. Binary Solvent Mixtures

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
310.95	0.9467	0.0537	331.85	0.8616	0.1384
316.25	0.9316	0.0684	336.45	0.8267	0.1733
321.75	0.9129	0.0871	341.45	0.7800	0.2200
327.35	0.8878	0.1122	346.25	0.7213	0.2787

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 97.9 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
306.2	0.9498	0.0502
319.8	0.9090	0.0910
331.8	0.8485	0.1515
342.2	0.7565	0.2435

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.1	0.9157	0.0843	353.0	0.5555	0.4445
321.3	0.8509	0.1491	366.2	0.3329	0.6671
331.6	0.7756	0.2244			
342.9	0.6856	0.3144			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.75	0.8335	0.1665	336.25	0.6475	0.3525
313.45	0.8050	0.1950	340.65	0.6043	0.3957
318.15	0.7785	0.2215	348.35	0.5256	0.4744
323.05	0.7472	0.2528	354.85	0.4523	0.5477
330.45	0.6945	0.3055			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 97.9 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and recrystallized from toluene.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:	EVALUATOR:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) Benzene; C_6H_6; [71-43-2]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

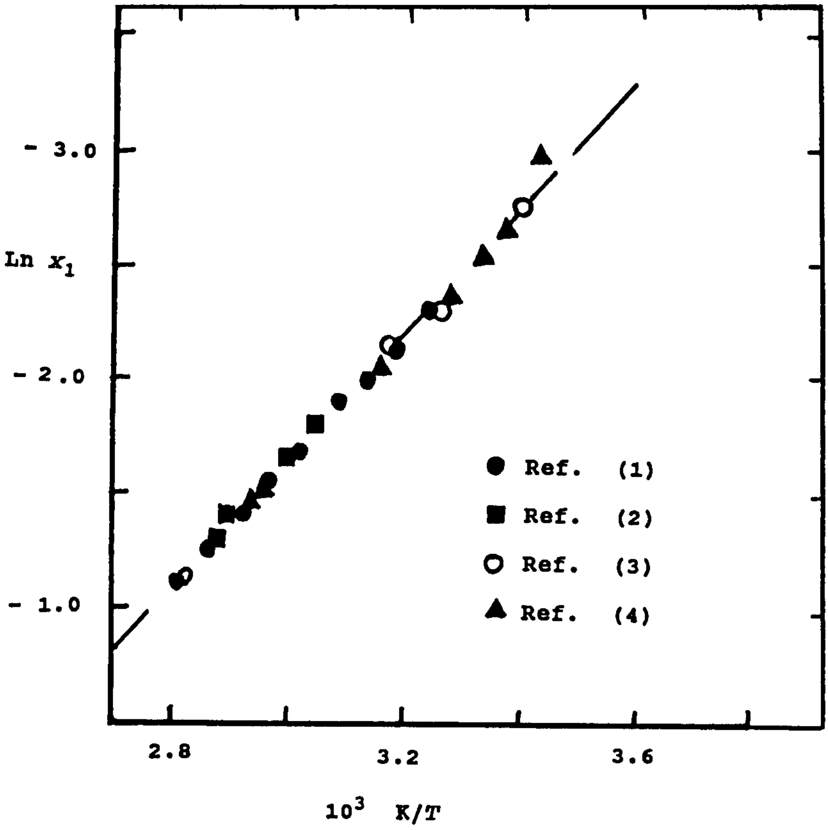
CRITICAL EVALUATION:

Fluorene solubilities in benzene were retrieved from papers by Choi *et al.* (1), McLaughlin and Zainal (2), Mortimer (3) and Domanska *et al.* (4). All four studies values at several temperatures. There is no a prior reason to exclude any of the four studies from the critical evaluation.

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

$$\text{Ln } x_1 = -2668.6 \, (1/T) + 6.8891 \qquad (r = 0.9995)$$

for variation of fluorene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

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

2. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1959, 863-867.

3. Mortimer, F.S. *J. Am. Chem. Soc.* 1923, *45*, 633-641.

4. Domanska, U.; Groves, F.R., Jr.; McLaughlin, E. *J. Chem. Eng. Data* 1993, *38*, 88-94.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.8	0.8396	0.1604	342.6	0.5941	0.4059
327.6	0.7222	0.2778	346.0	0.5595	0.4405
331.6	0.6905	0.3095			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.946	0.054	353	0.489	0.511
293	0.895	0.105			
313	0.810	0.190			
333	0.676	0.324			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Domanska, U.; Groves, F.R., Jr.; McLaughlin, E.

J. Chem. Eng. Data 1993, *38*, 88-94.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
278.7	1.0000	0.0000	(2)
277.5	0.9798	0.0202	(2)
277.0	0.9593	0.0407	(2)
275.8	0.9465	0.0535	(2)
275.3	0.9369	0.0631	(1)
278.1	0.9286	0.0714	(1)
283.1	0.9174	0.0826	(1)
288.9	0.9014	0.0986	(1)
290.7	0.8960	0.1040	(1)
295.0	0.8819	0.1181	(1)
298.4	0.8699	0.1301	(1)
304.7	0.8452	0.1548	(1)
308.7	0.8277	0.1723	(1)
315.2	0.7938	0.2062	(1)
324.5	0.7391	0.2609	(1)
331.6	0.6856	0.3144	(1)
337.5	0.6435	0.3565	(1)
339.7	0.6208	0.3792	(1)
344.5	0.5747	0.4253	(1)
347.7	0.5462	0.4538	(1)
349.2	0.5312	0.4688	(1)
388.0	0.0000	1.0000	(1)

Authors report eutectic point occurs at x_1 = 0.063 and T/K = 275.3.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) 99+ %, Aldrich Chemical Company, was fractionally distilled and stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) Methylbenzene; C_7H_8; [108-88-3]	Mortimer, F.S. *J. Am. Chem. Soc.* 1923, *45*, 633-641.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.946	0.054	353	0.489	0.511
293	0.894	0.106			
313	0.809	0.191			
333	0.676	0.324			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E. *Fluid Phase Equilibr.* 1989, *44*, 305-345.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
303.6	0.8328	0.1672	335.7	0.6298	0.3702
311.7	0.7925	0.2075	343.0	0.5666	0.4334
322.8	0.7305	0.2695	356.3	0.4272	0.5728
325.7	0.7139	0.2861			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.
(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS: (1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) Ethylbenzene; C_8H_{10}; [100-41-4]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M. *J. Appl. Chem. U.S.S.R.* 1952, *25*, 1015-1022. (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
178.8	1.000	0.000	(2)
178.2	0.990	0.010	Eutectic
209.2	0.979	0.021	(1)
253.2	0.951	0.046	(1)
281.8	0.900	0.100	(1)
308.4	0.801	0.199	(1)
325.9	0.702	0.298	(1)
339.0	0.602	0.398	(1)
349.2	0.498	0.502	(1)
357.2	0.404	0.596	(1)
365.9	0.300	0.700	(1)
374.2	0.182	0.818	(1)
379.5	0.102	0.898	(1)
387.2	0.000	1.000	(1)

Author reports eutectic point occurs at x_1 = 0.010 and T/K = 178.2.

AUXILIARY INFORMATION

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

(2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

J. Appl. Chem. U.S.S.R. 1952, *25*, 1015-1022 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
225.8	1.000	0.000	(2)
224.6	0.973	0.027	Eutectic
270.9	0.949	0.051	(1)
280.3	0.900	0.100	(1)
308.7	0.795	0.205	(1)
325.8	0.702	0.298	(1)
338.8	0.602	0.398	(1)
349.6	0.500	0.500	(1)
357.0	0.410	0.590	(1)
365.7	0.298	0.702	(1)
373.7	0.197	0.803	(1)
380.2	0.091	0.900	(1)
387.2	0.000	1.000	(1)

Author reports eutectic point occurs at x_1 = 0.027 and T/K = 224.6.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.945	0.055	353	0.487	0.513
293	0.888	0.112			
313	0.807	0.193			
333	0.673	0.327			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

(2) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

J. Appl. Chem. U.S.S.R. 1952, *25*, 1015-1022. (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
352.2	1.000	0.000	(2)
347.6	0.918	0.082	(2)
345.0	0.871	0.129	(2)
342.4	0.820	0.180	(2)
340.6	0.782	0.218	(2)
338.5	0.748	0.252	(2)
335.2	0.696	0.304	(2)
333.7	0.652	0.348	Eutectic
343.4	0.554	0.446	(1)
354.1	0.450	0.550	(1)
363.1	0.333	0.667	(1)
371.1	0.224	0.776	(1)
377.8	0.127	0.873	(1)
387.2	0.000	1.000	(1)

Author reports eutectic point occurs at $x_1 = 0.348$ and at $T/K = 333.7$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

J. Appl. Chem. U.S.S.R. 1952, *25*, 1015-1022. (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
353.2	1.000	0.000	(2)
347.5	0.921	0.079	(2)
342.4	0.844	0.156	(2)
335.7	0.755	0.245	(2)
329.4	0.658	0.342	(2)
328.2	0.625	0.375	(1)
329.7	0.612	0.388	(1)
337.0	0.564	0.436	(1)
348.7	0.466	0.534	(1)
358.6	0.359	0.641	(1)
368.5	0.247	0.753	(1)
377.6	0.121	0.879	(1)
387.2	0.000	1.000	(1)

Author reports eutectic point occurs at x_1 = 0.365 and T/K = 328.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS: (1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M. *J. Appl. Chem. U.S.S.R.* 1952, *25*, 1015-1022. (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
307.2	1.000	0.000	(2)
306.6	0.980	0.020	(2)
305.2	0.965	0.035	(2)
310.7	0.908	0.092	(1)
317.2	0.818	0.182	(1)
321.0	0.778	0.222	(1)
326.5	0.726	0.274	(1)
331.1	0.684	0.316	(1)
336.2	0.646	0.354	(1)
340.7	0.591	0.409	(1)
351.1	0.486	0.514	(1)
356.8	0.434	0.566	(1)
366.4	0.312	0.688	(1)
372.5	0.232	0.768	(1)
378.7	0.124	0.876	(1)
387.2	0.000	1.000	(1)

Compiler: Eutectic point occurs at about $x_1 = 0.038$ and T/K = 304.8.

AUXILIARY INFORMATION

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 2,7-Dimethylnaphthalene; $C_{12}H_{12}$; [582-16-1]	Kravchenko, V.M. *J. Appl. Chem. U.S.S.R.* 1952, *25*, 1015-1022. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
370.2	1.000	0.000	(2)
361.6	0.864	0.136	(2)
352.7	0.740	0.260	(2)
347.7	0.689	0.311	(2)
343.0	0.642	0.358	(2)
337.7	0.599	0.401	(2)
335.2	0.580	0.420	Eutectic
338.2	0.547	0.453	(1)
342.7	0.500	0.500	(1)
348.3	0.444	0.556	(1)
353.7	0.397	0.603	(1)
363.8	0.295	0.705	(1)
371.7	0.198	0.802	(1)
379.7	0.100	0.900	(1)
387.2	0.000	1.000	(1)

Author reports eutectic occurs at x_1 = 0.420 and at T/K = 335.2.

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.* 1939, *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) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) Fluoranthene; $C_{16}H_{10}$; [206-44-0]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
383.2	1.000	0.000	(2)
376.3	0.905	0.095	(2)
368.1	0.797	0.203	(2)
360.0	0.704	0.296	(2)
352.6	0.625	0.375	(2)
347.9	0.571	0.429	(2)
343.1	0.530	0.470	(2)
342.2	0.519	0.481	Eutectic
345.3	0.477	0.523	(1)
353.8	0.389	0.611	(1)
363.7	0.298	0.702	(1)
373.2	0.195	0.805	(1)
380.7	0.099	0.901	(1)
387.2	0.000	1.000	(1)

Authors report eutectic occurs at x_2 = 0.519 and T/K = 342.2.

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.* 1939, *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) Fluorene; $C_{16}H_{10}$; [86-73-7] (2) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S. *Zhur. Fiz. Khim.* 1957, *31*, 1802-1811.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
368.3	1.000	0.000	(2)
361.7	0.897	0.103	(2)
355.6	0.806	0.194	(2)
348.2	0.707	0.293	(2)
340.9	0.618	0.382	(2)
337.8	0.582	0.418	Eutectic
339.3	0.562	0.438	(1)
348.1	0.472	0.528	(1)
356.0	0.381	0.619	(1)
367.9	0.254	0.746	(1)
379.6	0.111	0.889	(1)
387.2	0.000	1.000	(1)

Authors report eutectic occurs at x_2 = 0.582 and at T/K = 337.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

(2) Chrysene; $C_{18}H_{12}$; [218-01-9]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
528.2	1.000	0.000	(2)
513.9	0.861	0.139	(2)
504.2	0.754	0.246	(2)
491.6	0.650	0.350	(2)
480.2	0.555	0.445	(2)
458.7	0.403	0.597	(2)
445.4	0.320	0.680	(2)
419.5	0.205	0.795	(2)
395.7	0.129	0.871	(2)
381.2	0.098	0.902	Eutectic
384.4	0.052	0.948	(1)
387.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
311.4	0.8381	0.1619	337.8	0.6564	0.3436
319.8	0.7931	0.2069			
326.0	0.7501	0.2499			
331.4	0.7121	0.2879			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.934	0.066	353	0.467	0.533
293	0.876	0.124			
313	0.786	0.214			
333	0.651	0.349			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
293	0.9965	0.0035
313	0.9942	0.0058
333	0.9890	0.0110

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
293	0.9950	0.0050
313	0.9915	0.0085
333	0.9824	0.0176
353	0.9540	0.0460

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.2082

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.937	0.063	353	0.475	0.525
293	0.882	0.118			
313	0.794	0.206			
333	0.659	0.341			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
311.5	0.8021	0.1979	359.2	0.3873	0.6127
327.1	0.7064	0.2936			
340.2	0.5998	0.4002			
349.0	0.5091	0.4909			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.949	0.051	353	0.501	0.499
293	0.899	0.101			
313	0.817	0.183			
333	0.686	0.314			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mortimer, F.S.

J. Am. Chem. Soc. 1923, *45*, 633-641.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273	0.976	0.024	353	0.573	0.427
293	0.944	0.056			
313	0.883	0.117			
333	0.768	0.232			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure not given in the reference. Compiler speculates that the experimental values were, in all likelihood, determined by a gravimetric method, which was common practice during this era. The method probably involved equilibrating excess solute and solvent in sealed containers, transfer of weighed aliquots of saturated solution to tared containers, evaporation of solvent, and weighing of solid residue that remained.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given. Paper states only that the solute was carefully purified.

(2) Purity and chemical source not given. Paper states only that the solvent was carefully purified.

ESTIMATED ERRORS:

T/K: ± 2 (by compiler).
x_1: ± 8 % (relative error, by compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
303.6	0.8156	0.1844	357.5	0.4046	0.5954
321.0	0.7238	0.2762			
335.5	0.6198	0.3802			
350.2	0.4854	0.5146			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 97.8 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 1,2-Dinitrobenzene; $C_6H_4N_2O_4$; [528-29-0]	Kremann, R. *Monatsch. Chem.* <u>1911</u>, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
388.2	1.000	0.000	(2)
385.0	0.931	0.069	(2)
382.8	0.872	0.128	(2)
378.2	0.785	0.215	(2)
371.2	0.701	0.299	(2)
365.7	0.629	0.371	(2)
361.6	0.576	0.424	(2)
356.4	0.518	0.482	(2)
352.3	0.457	0.543	(2)
357.2	0.393	0.607	(1)
365.2	0.299	0.701	(1)
371.2	0.217	0.783	(1)
375.2	0.163	0.837	(1)
378.2	0.114	0.886	(1)
382.2	0.060	0.940	(1)
385.7	0.000	1.000	(1)

Compiler: Eutectic point occurs at about $x_1 = 0.548$ and T/K = 351.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

(2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1911, *32*, 609-617.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
362.2	1.000	0.000	(2)
357.7	0.929	0.071	(2)
352.7	0.837	0.163	(2)
345.7	0.764	0.236	(2)
339.7	0.672	0.328	(2)
332.2	0.606	0.394	(2)
329.2	0.579	0.421	Eutectic
332.7	0.547	0.453	(1)
338.2	0.511	0.489	(1)
341.7	0.485	0.515	(1)
345.7	0.466	0.534	(1)
350.7	0.415	0.585	(1)
356.2	0.370	0.630	(1)
362.7	0.315	0.685	(1)
365.2	0.260	0.740	(1)
374.7	0.152	0.848	(1)
378.2	0.104	0.896	(1)
382.2	0.050	0.950	(1)
385.7	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 1,4-Dinitrobenzene; $C_6H_4N_2O_4$; [100-25-4]	Kremann, R. *Monatsch. Chem.* 1911, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
445.2	1.000	0.000	(2)
437.2	0.871	0.129	(2)
431.2	0.792	0.208	(2)
425.2	0.714	0.286	(2)
413.2	0.581	0.419	(2)
395.2	0.431	0.569	(2)
389.2	0.396	0.606	(2)
382.7	0.359	0.641	(2)
376.7	0.329	0.671	(2)
368.7	0.298	0.702	(2)
364.7	0.259	0.741	(1)
366.2	0.238	0.762	(1)
368.2	0.220	0.780	(1)
376.2	0.131	0.869	(1)
380.2	0.080	0.920	(1)
384.2	0.028	0.972	(1)
387.7	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.729 and at T/K = 363.1.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 1,3,5-Trinitrobenzene; $C_6H_3N_3O_6$; [99-35-4]	Kremann, R. *Monatsch. Chem.* 1911, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
394.2	1.000	0.000	(2)
392.7	0.963	0.037	(2)
385.7	0.895	0.105	(2)
378.2	0.801	0.199	(2)
373.7	0.732	0.268	1:1 Compound
377.7	0.666	0.334	1:1 Compound
378.2	0.611	0.389	1:1 Compound
377.2	0.563	0.437	1:1 Compound
376.2	0.514	0.486	1:1 Compound
374.2	0.456	0.544	1:1 Compound
371.2	0.407	0.593	1:1 Compound
369.2	0.387	0.613	1:1 Compound
366.2	0.351	0.649	1:1 Compound
360.2	0.314	0.686	1:1 Compound
363.7	0.256	0.744	(1)
369.2	0.195	0.805	(1)
374.2	0.139	0.861	(1)
379.2	0.076	0.924	(1)
382.2	0.034	0.966	(1)
385.7	0.000	1.000	(1)

Compiler: Phase diagram indicates formation of a 1:1 fluorene - 1,3,5-trinitrobenzene molecular compound, with the two eutectic points at about x_1 = 0.252 and *T*/K = 373.2, and at x_1 = 0.700 and *T*/K = 358.8.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.5 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 1,2,3,5-Tetranitrobenzene; $C_6H_2N_4O_8$; [3698-53-1]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
399.2	1.000	0.000	(2)
393.7	0.903	0.097	(2)
398.2	0.824	0.176	1:2 Compound
402.2	0.725	0.275	1:2 Compound
403.2	0.674	0.326	1:2 Compound
403.2	0.649	0.351	1:2 Compound
402.2	0.606	0.394	1:2 Compound
402.7	0.602	0.398	1:2 Compound
401.5	0.543	0.457	1:2 Compound
397.7	0.450	0.550	1:2 Compound
381.2	0.272	0.728	1:2 Compound
370.2	0.231	0.769	1:2 Compound
373.4	0.170	0.830	(1)
382.2	0.086	0.914	(1)
389.2	0.000	1.000	(1)

Author reports formation of a 1:2 fluorene - 1,2,3,5-tetranitrobenzene orangish-red compound having a melting point temperature of 403.2 K. Two eutectic points occur at x_1 = 0.120 and T/K = 390.7, and at x_1 = 0.780 and T/K = 364.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 2,4-Dinitro-1-methylbenzene; $C_7H_6N_2O_4$; [121-14-2]	Kremann, R. *Monatsch. Chem.* <u>1911</u>, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
341.2	1.000	0.000	(2)
338.2	0.913	0.087	(2)
329.2	0.732	0.268	(2)
319.2	0.614	0.386	(2)
318.8	0.585	0.415	(1)
329.2	0.536	0.464	(1)
340.2	0.474	0.526	(1)
349.7	0.402	0.598	(1)
357.2	0.345	0.655	(1)
366.4	0.238	0.762	(1)
372.2	0.167	0.833	(1)
385.7	0.000	1.000	(1)

Compiler: Eutectic point occurs at about $x_1 = 0.408$ and $T/\text{K} = 317.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 2,4,6-Trinitro-1-methylbenzene; $C_7H_5N_3O_6$; [118-96-7]	Kremann, R. *Monatsch. Chem.* <u>1911</u>, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
355.2	1.000	0.000	(2)
348.7	0.859	0.141	(2)
350.2	0.736	0.264	1:1 Compound
354.2	0.689	0.311	1:1 Compound
356.2	0.643	0.357	1:1 Compound
357.7	0.590	0.410	1:1 Compound
357.7	0.536	0.464	1:1 Compound
358.2	0.517	0.483	1:1 Compound
358.2	0.493	0.507	1:1 Compound
357.7	0.467	0.533	1:1 Compound
357.2	0.436	0.564	1:1 Compound
355.7	0.399	0.601	1:1 Compound
354.2	0.371	0.629	1:1 Compound
354.2	0.336	0.664	1:1 Compound
356.7	0.308	0.692	1:1 Compound
364.2	0.248	0.752	(1)
372.2	0.168	0.832	(1)
376.2	0.114	0.886	(1)
383.0	0.077	0.923	(1)
385.7	0.000	1.000	(1)

Compiler: Phase diagram indicates formation of a 1:1 fluorene - 2,4,6-trinitromethylbenzene molecular compound melting at about T/K = 358.5. Two eutectic points occur at about x_1 = 0.22 and T/K = 345.5 and at x_1 = 0.71 and T/K = 353.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 2,4-Dinitrophenol; $C_6H_4N_2O_5$; [51-28-5]	Kremann, R. *Monatsch. Chem.* 1911, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
385.2	1.000	0.000	(2)
378.2	0.872	0.128	(2)
373.2	0.775	0.225	(2)
368.7	0.711	0.289	(2)
365.2	0.660	0.340	(2)
362.7	0.620	0.380	(2)
358.7	0.579	0.421	(2)
355.2	0.538	0.462	(2)
352.2	0.512	0.488	(2)
350.2	0.488	0.512	(2)
349.7	0.484	0.516	(2)
348.2	0.466	0.534	(2)
347.2	0.455	0.545	Eutectic
349.2	0.431	0.569	(1)
350.7	0.427	0.573	(1)
352.2	0.409	0.591	(1)
355.7	0.376	0.624	(1)
363.2	0.304	0.696	(1)
375.2	0.177	0.823	(1)
385.7	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) 2,4,6-Trinitrophenol; $C_6H_3N_3O_7$; [88-89-1]	Kremann, R. *Monatsch. Chem.* 1911, *32*, 609-617.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
395.2	1.000	0.000	(2)
384.2	0.866	0.134	(2)
376.2	0.771	0.229	(2)
369.2	0.707	0.293	(2)
357.2	0.605	0.395	(2)
355.2	0.554	0.446	1:1 Compound
356.7	0.522	0.478	1:1 Compound
357.2	0.474	0.526	1:1 Compound
357.2	0.434	0.566	1:1 Compound
355.2	0.394	0.606	1:1 Compound
354.2	0.362	0.638	Eutectic (?)
359.2	0.297	0.703	(1)
365.7	0.234	0.766	(1)
372.2	0.168	0.832	(1)
378.7	0.103	0.897	(1)
383.2	0.041	0.959	(1)
385.7	0.000	1.000	(1)

Compiler: Phase diagram shows formation of a 1:1 molecular compound melting at about $T/K = 377.5$. Two eutectic points occur at about $x_1 = 0.42$ and $T/K = 353.4$ and at $x_1 = 0.64$ and $T/K = 353.8$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

(2) 6-Methyl-2,3,4-trinitrophenol; $C_7H_5N_3O_7$; [89793-90-8]

ORIGINAL MEASUREMENTS:

Efremov, N.N.; Fikhomirova, A.N.

J. Russ. Phys. Chem. Soc. 1927, *57*, 373-390.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase equilibrium data not given in cited paper. Authors report formation of a 1:1 fluorene - 6-methyl-2,3,4-trinitrophenol molecular compound. The two eutectic points occur at x_1 = 0.190 and T/K = 358.6 and at x_1 = 0.751 and T/K = 363.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental details not given in paper.

determined using a Toshiniwal Melting Point Apparatus equipped with a precision thermometer.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.003 (Compiler).

INDOLE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

benzene
biphenyl
1-methylnaphthalene
2-methylnaphthalene
2,6-dimethylnaphthalene

D. Esters

E. Ethers

diphenyl ether

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

ethanol

H. Ketones

I. Miscellaneous Pure Solvents

quinoline
2-methylindole
5-methylindole

J. Binary Solvent Mixtures

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Indole; C_8H_7N; [120-72-9] (2) Benzene; C_6H_6; [71-43-2]	Yokoyama, C.; Ebina, T.; Takahashi, S. *J. Chem. Eng. Data* <u>1993</u>, *38*, 583-586.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
278.73	1.0000	0.0000	(2)
275.05	0.9479	0.0521	(2)
268.31	0.8000	0.2000	(2)
266.37	0.7490	0.2510	(2)
269.32	0.7190	0.2810	(1)
274.58	0.6510	0.3490	(1)
279.40	0.5990	0.4010	(1)
288.54	0.4990	0.5010	(1)
303.68	0.2850	0.7150	(1)
309.88	0.2080	0.7920	(1)
317.59	0.0980	0.9020	(1)
326.26	0.0000	1.0000	(1)

Authors report eutectic occurs at x_1 = 0.2552 and at T/K = 265.90.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

(2) 99.9 %, Wako Pure Chemical Ind Ltd., was dried over molecular sieves prior to use.

ESTIMATED ERRORS:

T/K: precision ± 0.02.
x_1: ± 0.0001.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Indole; C_8H_7N; [120-72-9] (2) Biphenyl; $C_{12}H_{10}$; [92-52-4]	Yokoyama, C.; Ebina, T.; Takahashi, S. *J. Chem. Eng. Data* 1993, *38*, 583-586.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
343.13	1.0000	0.0000	(2)
335.36	0.8564	0.1436	(2)
328.51	0.7136	0.2864	(2)
323.66	0.6291	0.3709	(2)
318.19	0.5363	0.4637	(2)
312.57	0.4435	0.5565	(2)
308.08	0.3902	0.6098	(2)
304.01	0.3462	0.6538	(2)
301.45	0.3174	0.6826	(1)
301.76	0.3005	0.6995	(1)
306.45	0.2470	0.7530	(1)
310.08	0.1998	0.8002	(1)
317.55	0.1022	0.8978	(1)
326.26	0.0000	1.0000	(1)

Authors report eutectic occurs at x_1 = 0.6815 and at T/K = 300.71.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

(2) 99.8 %, Wako Pure Chemical Ind Ltd., was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.02.
x_1: ± 0.0001.

COMPONENTS:

(1) Indole; C_8H_7N; [120-72-9]

(2) Biphenyl; $C_{12}H_{10}$; [92-52-4]

ORIGINAL MEASUREMENTS:

Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.

Int. DATA Ser., Ser. A 1984, 46.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
341.99	1.0000	0.0000	(2)
337.00	0.8973	0.1027	(2)
335.75	0.8724	0.1276	(2)
333.90	0.8356	0.1644	(2)
329.75	0.7524	0.2476	(2)
323.85	0.6393	0.3607	(2)
317.65	0.5326	0.4674	(2)
310.95	0.4317	0.5683	(2)
302.70	0.3362	0.6638	(2)
302.05	0.3055	0.6945	(1)
306.45	0.2456	0.7544	(1)
312.65	0.1596	0.8404	(1)
318.75	0.0778	0.9222	(1)
324.95	0.0000	1.0000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Pure Grade, Inst. Chem. Przerobki Wegla, Zabrze, Poland, was recrystallized thrice from methanol.

(2) Pure Grade, Glovkhimreaktiv, Khartov, USSR, was recrystallized thrice from methanol and zone refined.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0005.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Indole; C_8H_7N; [120-72-9] (2) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]	Yokoyama, C.; Ebina, T.; Takahashi, S. *J. Chem. Eng. Data* 1993, *38*, 583-586.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
242.45	1.0000	0.0000	(2)
239.55	0.9660	0.0340	(2)
239.57	0.9586	0.0414	(2)
237.20	0.9308	0.0692	(2)
236.00	0.9088	0.0912	(2)
237.78	0.8973	0.1027	(1)
253.91	0.8292	0.1708	(1)
266.53	0.7440	0.2560	(1)
271.73	0.6980	0.3020	(1)
280.09	0.6048	0.3952	(1)
300.43	0.4048	0.5952	(1)
311.68	0.2018	0.7982	(1)
319.24	0.0773	0.9227	(1)
326.26	0.0000	1.0000	(1)

Authors report eutectic occurs at x_1 = 0.0946 and at T/K = 235.31.

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 visual noting the temperature at which the last trace of solid solute disappeared.	(1) 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received. (2) 99.9 %, Aldrich Chemical Comapny, was dried over molecular sieves prior to use. **ESTIMATED ERRORS:** T/K: precision ± 0.02. x_1: ± 0.0001.

COMPONENTS:

(1) Indole; C_8H_7N; [120-72-9]

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

ORIGINAL MEASUREMENTS:

Yokoyama, C.; Ebina, T.; Takahashi, S.

J. Chem. Eng. Data 1993, *38*, 583-586.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
307.09	1.0000	0.0000	(2)
299.28	0.8566	0.1434	(2)
295.28	0.7821	0.2179	(2)
290.53	0.6832	0.3168	(2)
286.44	0.6151	0.3849	(2)
283.13	0.5574	0.4426	(1)
286.75	0.5024	0.4976	(1)
296.06	0.3964	0.6036	(1)
303.62	0.2962	0.7038	(1)
310.38	0.2030	0.7970	(1)
317.82	0.1007	0.8993	(1)
326.26	0.0000	1.0000	(1)

Authors report eutectic occurs at $x_1 = 0.4373$ and at $T/K = 282.77$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

(2) 99.8 %, Aldrich Chemical Comapny, was used as received from manufacturer.

ESTIMATED ERRORS:

T/K: precision ± 0.02.
x_1: ± 0.0001.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Indole; C_8H_7N; [120-72-9] (2) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]	Szafranski, A.M.; Wyrzykowska-Stankiewicz, D. *Int. DATA Ser., Ser. A* 1984, 48.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
307.69	1.0000	0.0000	(2)
301.75	0.8812	0.1188	(2)
296.05	0.7672	0.2328	(2)
290.45	0.6578	0.3422	(2)
284.75	0.5527	0.4473	(2)
284.50	0.5322	0.4678	(1)
285.65	0.5185	0.4815	(1)
290.65	0.4517	0.5483	(1)
298.65	0.3545	0.6455	(1)
305.55	0.2609	0.7391	(1)
311.95	0.1708	0.8292	(1)
318.35	0.0839	0.9161	(1)
324.95	0.0000	1.0000	(1)

Compiler: Eutectic point occurs at about $x_1 = 0.466$ and $T/K = 284.3$..

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.	(1) Pure Grade, Inst. Chem. Przerobki Wegla, Zabrze, Poland, was recrystallized thrice from aqueous-methanol. (2) Pure Grade, Inst. Chem. Przerobki Wegla, was recrystallized thrice from methanol. **ESTIMATED ERRORS:** T/K: precision ± 0.1. x_1: ± 0.0005.

COMPONENTS:

(1) Indole; C_8H_7N; [120-72-9]

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

ORIGINAL MEASUREMENTS:

Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.

Int. DATA Ser., Ser. A 1984, 49.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
383.35	1.0000	0.0000	(2)
376.75	0.8709	0.1291	(2)
371.75	0.7497	0.2503	(2)
360.35	0.5294	0.4706	(2)
354.35	0.4285	0.5715	(2)
347.55	0.3333	0.6667	(2)
338.55	0.2432	0.7568	(2)
327.25	0.1579	0.8421	(2)
318.15	0.1169	0.8831	(2)
316.15	0.1100	0.8900	Eutectic
316.95	0.1034	0.8966	(1)
317.95	0.0901	0.9099	(1)
318.75	0.0769	0.9231	(1)
324.95	0.0000	1.0000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.8900 and T/K = 316.15.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Pure Grade, Inst. Chem. Przerobki Wegla, Zabrze, Poland, was recrystallized thrice from aqueous-methanol.

(2) Pure Grade, Schuchardt, Munchen, GFR, was sodium-refined and fractionally crystallized.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0005.

COMPONENTS:

(1) Indole; C_8H_7N; [120-72-9]

(2) Diphenyl ether; $C_{12}H_{10}O$; [101-84-8]

ORIGINAL MEASUREMENTS:

Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.

Int. DATA Ser., Ser. A 1984, 50.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
300.00	1.0000	0.0000	(2)
294.15	0.8610	0.1390	(2)
291.55	0.7959	0.2041	(2)
289.05	0.7336	0.2664	(2)
283.75	0.6163	0.3837	(2)
282.35	0.5884	0.4116	(2)
281.75	0.5611	0.4389	(1)
286.15	0.5080	0.4920	(1)
294.55	0.4077	0.5923	(1)
301.15	0.3145	0.6855	(1)
307.95	0.2278	0.7722	(1)
313.85	0.1468	0.8532	(1)
324.95	0.0000	1.0000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.433 and at T/K = 281.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Pure Grade, Inst. Chem. Przerobki Wegla, Zabrze, Poland, was recrystallized thrice from aqueous-methanol.

(2) Pure Grade, Fabryka Odczynnikow Chem., Gliwice, Poland, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0005.

COMPONENTS: (1) Indole; C_8H_7N; [120-72-9] (2) Ethanol; C_2H_6O; [64-17-5]	**ORIGINAL MEASUREMENTS:** Pucher, G.; Dehn, W.M. *J. Am. Chem. Soc.* 1921, *43*, 1753-1758.
VARIABLES: Ambient Room Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2^a	x_1^a
0.876	0.124

[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

Excess solute and solvent equilibrated at ambient room temperature. Solution was filtered rapidly into a tared crucible. Solvent was evaporated. Solubility determined from weights of solid residue and evaporated solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given, was used as received.

(2) Absolute, chemical source not given, was dried over calcium carbide and distilled before use.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS: (1) Indole; C_8H_7N; [120-72-9] (2) Quinoline; C_9H_7N; [91-22-5]	**ORIGINAL MEASUREMENTS:** Pucher, G.; Dehn, W.M. *J. Am. Chem. Soc.* 1921, *43*, 1753-1758.
VARIABLES: Ambient Room Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2^a	x_1^a
0.888	0.112

[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

Excess solute and solvent equilibrated at ambient room temperature. Solution was filtered rapidly into a tared crucible. Solvent was evaporated. Solubility determined from weights of solid residue and evaporated solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given, was used as received.

(2) Purity and chemical source not given, was dried over potassium hydroxide and and sodium metal and distilled

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Indole; C_8H_7N; [120-72-9]

(2) 2-Methylindole; C_9H_9N; [95-20-5]

ORIGINAL MEASUREMENTS:

Yokoyama, C.; Ebina, T.; Takahashi, S.

J. Chem. Eng. Data 1993, *38*, 583-586.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
332.77	1.0000	0.0000	(2)
325.03	0.8875	0.1125	(2)
318.87	0.7974	0.2026	(2)
311.01	0.6988	0.3012	(2)
302.02	0.5982	0.4018	(2)
292.89	0.5001	0.4999	(2)
289.52	0.3995	0.6005	(1)
300.39	0.2985	0.7015	(1)
310.05	0.1999	0.8001	(1)
318.18	0.0967	0.9033	(1)
326.26	0.0000	1.0000	(1)

Authors report eutectic occurs at $x_1 = 0.5621$ and at T/K = 286.24.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

(2) 99.0 %, Aldrich Chemical Comapny, was used as received from manufacturer.

ESTIMATED ERRORS:

T/K: precision ± 0.02.
x_1: ± 0.0001.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Indole; C_8H_7N; [120-72-9] (2) 5-Methylindole; C_9H_9N; [614-96-0]	Yokoyama, C.; Ebina, T.; Takahashi, S. *J. Chem. Eng. Data* 1993, *38*, 583-586.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
333.74	1.0000	0.0000	(2)
327.70	0.8949	0.1051	(2)
321.45	0.7994	0.2006	(2)
315.52	0.6979	0.3021	(2)
307.85	0.6002	0.3998	(2)
298.72	0.4993	0.5007	(2)
289.20	0.4010	0.5990	(1)
300.78	0.2994	0.7006	(1)
310.37	0.2001	0.7999	(1)
317.99	0.1004	0.8996	(1)
326.26	0.0000	1.0000	(1)

Authors report eutectic occurs at x_1 = 0.5915 and at *T*/K = 289.63.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

(2) 99.0 %, Aldrich Chemical Comapny, was used as received from manufacturer.

ESTIMATED ERRORS:

T/K: precision ± 0.02.
x_1: ± 0.0001.

NAPHTHACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

benzene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:

(1) Naphthacene; $C_{18}H_{12}$; [92-24-0]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.00016

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Naphthacene; $C_{18}H_{12}$; [92-24-0]

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

ORIGINAL MEASUREMENTS:

Mishra, D.S.; Yalkowsky, S.H.

Ind. Eng. Chem. Res., 1990, *29*, 2278-2283.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
23.0	0.9857	0.0143

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in screw-capped test tube and allowed to equilibrate for 3 days with gentle agitation in a constant temperature bath. Samples centrifuged for 30 minutes and concentrations were determined spectrophotometrically. Attainment of equilibrium verified by repetitive measurements 4 days later.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent grade, source not specified, was used as received.

(2) Reagent grade, source not specified, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D. *Environ. Sci. Technol.* 1985, *19*, 522-529.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.00530

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

NAPHTHALENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
n-hexadecane
n-octadecane
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
1,2-dimethylbenzene
1,3-dimethylbenzene
1,4-dimethylbenzene
biphenyl
1,2-diphenylethane
1,2,3,4-tetrahydronaphthalene
4-isopropyl methylbenzene
indene
fluoranthene
fluorene
chrysene
pyrene
acenaphthene

D. Esters

furfuryl acetate
methyl 2-furoate
ethyl 2-furoate
n-propyl 2-furoate
n-butyl 2-furoate

E. Ethers

1,1-oxybisethane
1,1-oxybisbutane
1-ethoxypropane
2-ethoxypropane
2,2-dimethyloxetane
3,3-dimethyloxetane
tetrahydropyran

F. Haloalkanes and Haloaromatic Hydrocarbons

dichloromethane
trichloromethane
tetrachloromethane
trichloroethylene
diiodomethane
1,1-dibromoethane
1,2-dibromoethane
1,1-dichloroethane
1,2-dichloroethane
chlorobenzene
1,4-dichlorobenzene
hexafluorobenzene
octafluoronaphthalene

G. Alcohols

methanol
ethanol
1-propanol
2-propanol
1-butanol
2-butanol
2-methyl-1-propanol
2-methyl-2-propanol
1-pentanol
1-hexanol
1-octanol
cyclohexanol
methylcyclohexanol
1,4-benzenediol
1,2-benzenediol
1,3-benzenediol
furfuryl alcohol

H. Ketones

2-propanone

I. Miscellaneous Pure Solvents

carbon disulfide
nitrobenzene
aniline
thiophene
pyridine
2-nitrobenzaldehyde
3-nitrobenzaldehyde
4-nitrobenzaldehyde
1-chloro-3-nitrobenzene
1-chloro-4-nitrobenzene
2,4-dinitroaniline
3,5-dinitrobenzoic acid
1,3,5-trimethyl-2,4,6-trinitrobenzene
4-nitro-1-methylbenzene
1,3-dinitrobenzene

1,3,5-trinitrobenzene
2-nitrophenol
4-nitrophenol
2,4-dinitro-1-methylbenzene
2,4-dinitrophenol
2,4,6-trinitrophenol
isoquinoline
perfluoro-dibutyl ether
perfluoro-tripropylamine

J. Binary Solvent Mixtures

benzene + methylbenzene
benzene + 1,3-dimethylbenzene
benzene + isoquinoline
acetonitrile + water
methanol + water
1-propanol + water
1-hexanol + water
2-propanone + water
2-butanone + water
1,2-ethanediol + water
ethyl ethanoate + water
pyridine + water

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) n-Hexane; C_6H_{14}; [110-54-3]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

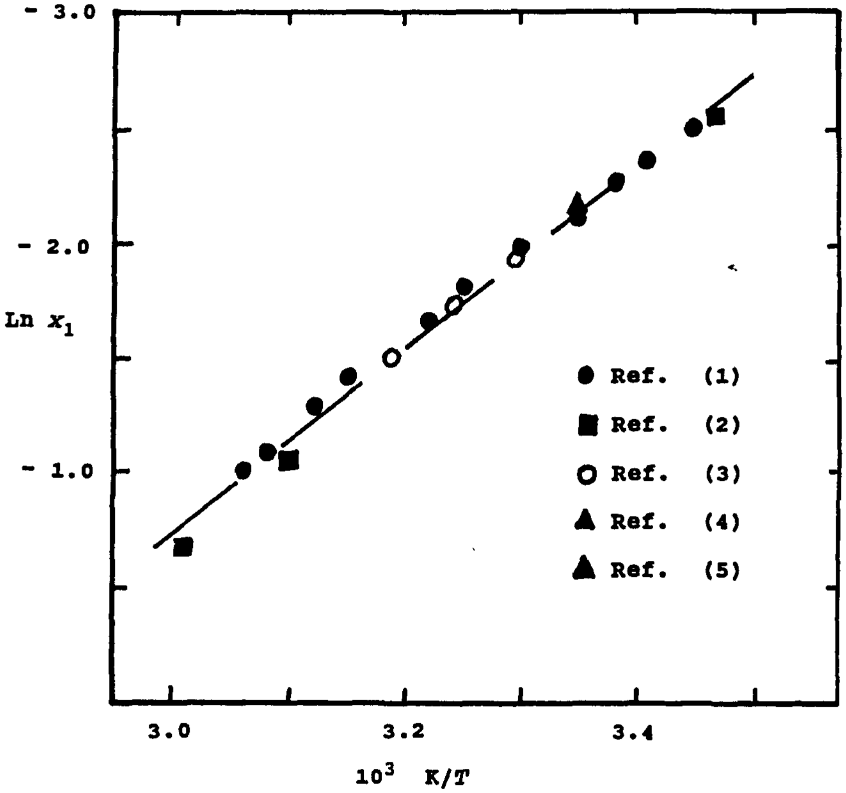
CRITICAL EVALUATION:

Naphthalene solubilities in n-hexane were retrieved from papers by Domanska (1), Ward (2), Acree *et al.* (3), Heric and Posey (4), and Chang (5). The first two studies report values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and both Heric and Posey 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:

$$\mathrm{Ln}\ x_1 = -3849.6\ (1/T) + 10.789 \qquad (r = 0.9964)$$

for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Domanska, U. *Polish J. Chem.* <u>1981</u>, *55*, 1715-1720.
2. Ward, H.L. *J. Phys. Chem.* <u>1926</u>, *30*, 1316-1333.
3. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* <u>1986</u>, *31*, 225-230.
4. Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* <u>1964</u>, *9*, 35-43.
5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.8832	0.1168

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.878	0.122

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Domanska, U.

Polish J. Chem. 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
282.05	0.937	0.063
286.35	0.928	0.072
289.55	0.916	0.084
289.85	0.918	0.082
292.45	0.906	0.094
295.45	0.894	0.104
298.65	0.881	0.119
302.45	0.862	0.138
306.75	0,837	0.163
310.25	0.811	0.189
317.05	0.757	0.243
319.25	0.723	0.277
319.65	0.724	0.276
324.15	0.660	0.340
325.75	0,632	0.368

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Reachim, Poland, was dried over phosphorous pentoxide and fractionally distilled to a final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
288.0	0.921	0.0792	331.6	0.492	0.508
301.7	0.865	0.135			
322.8	0.661	0.339			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Purity not given, Eastman Kodak Company, Rochester, New York, USA, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. 1986, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.8585	0.1415	40.0	0.7784	0.2216
35.0	0.8237	0.1763			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and gas chromatograph.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

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

ESTIMATED ERRORS:

T/K: ± 0.05.

x_1: ± 1 % (relative error).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.870	0.130

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.60

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.858	0.142

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.7957	0.2043

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Practical Grade, Eastman Chemical Company, was dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Djordjevic, N.M.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
325.1	0.4776	0.5224	346.0	0.1350	0.8650
330.0	0.4044	0.5956	347.0	0.1150	0.8850
342.5	0.2004	0.7996	348.7	0.0816	0.9184

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. 1986, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.8175	0.1825	40.0	0.7233	0.2767
35.0	0.7749	0.2251			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and gas chromatograph.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

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

ESTIMATED ERRORS:

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

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Cyclohexane; C_6H_{12}; [110-82-7]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

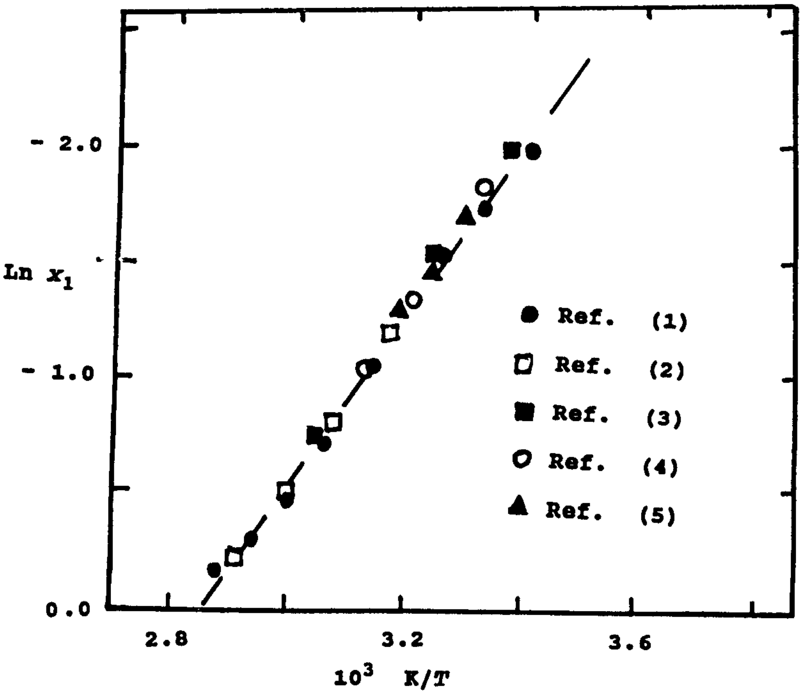
CRITICAL EVALUATION:

Naphthalene solubilities in cyclohexane were retrieved from papers by Heric and Yeh (1), Choi *et al.* (2), Domanska (3), McLaughlin (4), Acree *et al.* (5), Heric and Posey (6) and Chang (7). The first four studies report solubilities at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and the latter two studies measured the mole fraction solubility at a single temperature of 298 K. There is no a prior reason to exclude any of the seven studies from the critical evaluation.

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

$$\text{Ln } x_1 = -3916.1\ (1/T) + 11.2291 \qquad (r = 0.9984)$$

for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus $1/T$

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1. Heric, E.L.; Yeh, K.-N. *J. Chem. Eng. Data* 1970, *15*, 13-17.
2. Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. *J. Chem. Eng. Data* 1985, *30*, 403-409.
3. Domanska, U. *Polish J. Chem.* 1981, *55*, 1715-1720.
4. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 3854-3857.
5. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
6. Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1964, *9*, 35-43.
7. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.8513	0.1487

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.8 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E. L; Yeh, K.-N.

J. Chem. Eng. Data 1970, *15*, 13-17.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
292.95	0.8655	0.1345	326.75	0.5151	0.4849
301.83	0.8280	0.1720	334.01	0.3756	0.6244
306.71	0.7878	0.2122	340.06	0.2545	0.7455
318.28	0.6537	0.3463	346.75	0.1238	0.8762

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, Baker Chemical Company, USA, was used as received.

(2) Reagent Grade, Baker Chemical Company, was stored over phosphorous pentoxide and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.03.
x_1: ± 0.0001.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data <u>1985</u>, *30*, 403-409.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.15	0.8403	0.1597	325.45	0.5388	0.4612
308.25	0.7746	0.2254	333.15	0.3927	0.6073
315.15	0.6975	0.3025	343.05	0.1918	0.8082

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Naphthalene; C_8H_{10}; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Domanska, U.
Polish J. Chem. <u>1981</u>, *55*, 1715-1720.
(numerical values obtained through personal communication with author.)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
326.75	0.515	0.485	301.85	0.828	0.172
319.40	0.642	0.358	301.55	0.830	0.170
318.25	0.654	0.346	295.95	0.866	0.134
306.75	0.788	0.212	295.50	0.869	0.131
306.35	0.792	0.208			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, P.O.Ch., was dried over sodium metal and fractionally distilled to 99.9+ % purity.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.853	0.147

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Naphthalene; $C_{10}H$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.2	0.8459	0.1541	329.6	0.4620	0.5380
311.2	0.7480	0.2520			
318.8	0.6521	0.3479			
325.4	0.5424	0.4576			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.853	0.147

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.837	0.163

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

(2) trans-1,2-Dimethylcyclohexane; C_8H_{16}; [6876-23-9]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.847	0.153

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

(2) trans-1,4-Dimethylcyclohexane; C_8H_{16}; [2207-04-7]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.850	0.150

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

(2) cis-1,4-Dimethylcyclohexane; C_8H_{16}; [624-29-3]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.847	0.153

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

(2) cis-1,3-Dimethylcyclohexane; C_8H_{16}; [638-04-0]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.845	0.155

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. <u>1989</u>, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
302.9	0.7738	0.2262	324.3	0.5297	0.4703
307.7	0.7295	0.2705	329.7	0.4377	0.5623
311.7	0.6819	0.3181	335.6	0.3275	0.6725
319.0	0.6040	0.3960			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. <u>1986</u>, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.6682	0.3318	40.0	0.5757	0.4243
35.0	0.6211	0.3789			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and gas chromatograph.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

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

ESTIMATED ERRORS:

T/K: ± 0.05.

x_1: ± 1 % (relative error).

COMPONENTS:	**EVALUATOR:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Benzene; C_6H_6; [71-43-2]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

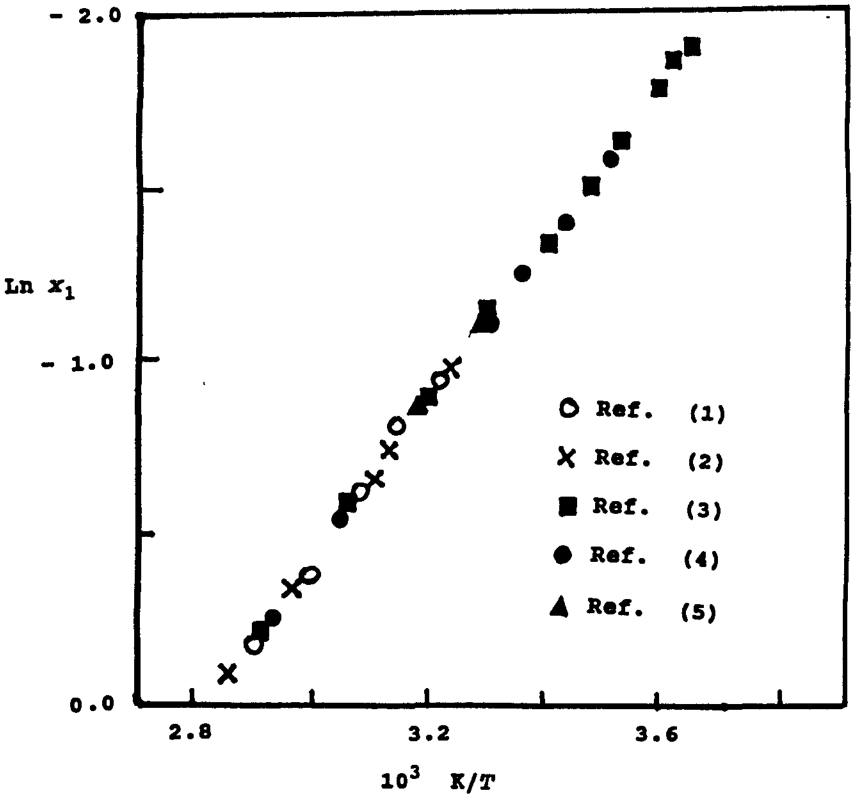
CRITICAL EVALUATION:

Naphthalene solubilities in benzene were retrieved from papers by Choi *et al.* (1), McLaughlin and Zainal (2), Ward (3), Kravchenko (4), Acree *et al.* (5), Heric and Posey (6) and Chang (7). The first four studies report values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and both Heric and Posey and Chang measured the mole fraction solubility at the single temperature of 298 K. There is no a prior reason to exclude any of the six studies from the critical evaluation.

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

$$\text{Ln } x_1 = -2301.9\ (1/T) + 6.5066 \qquad (r = 0.9996)$$

for variation of naphthalene solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.2974$, and differs by less than 2 % from experimental values of $x_1 = 0.2946$ (6) and $x_1 = 0.292$ (7).



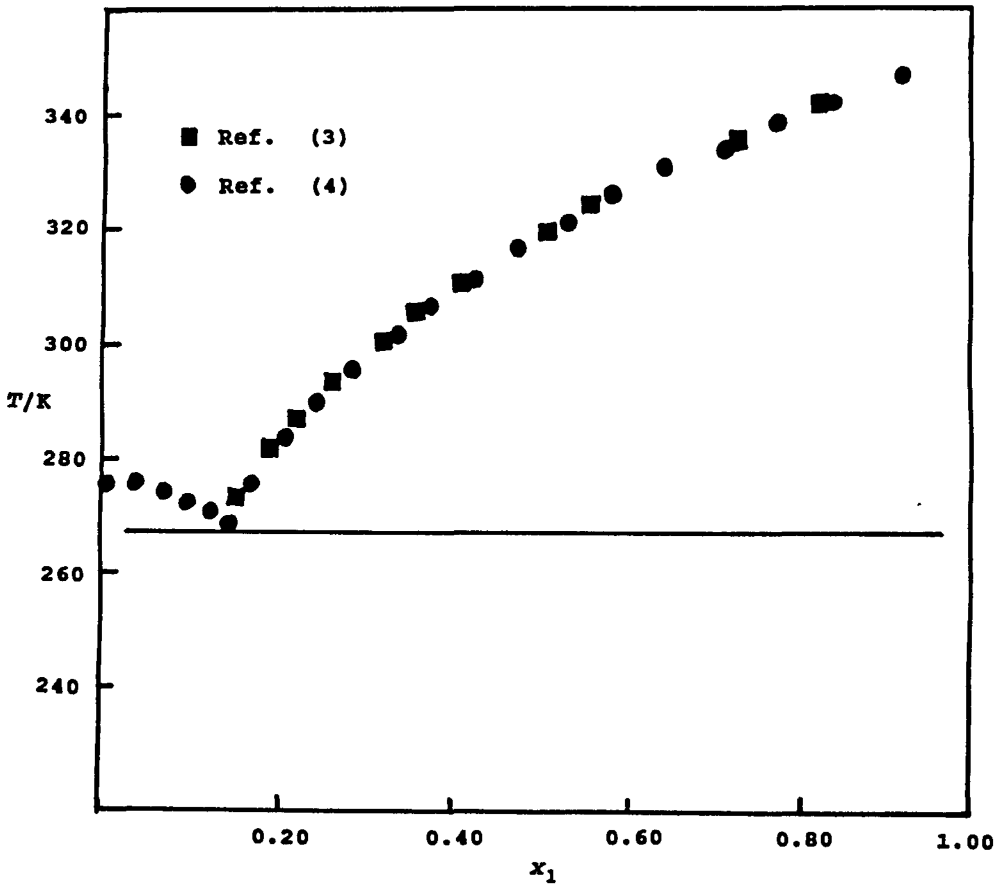
Graphical plot of Ln x_1 versus $1/T$

(Continued on next page)

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Benzene; C_6H_6; [71-43-2]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

CRITICAL EVALUATION: (Continued from previous page)

Experimental data from papers by Ward and Kravchenko were used to construct the phase diagram shown below. Binary mixtures of naphthalene and benzene exhibit a simple eutectic system.



Phase Diagram of the Naphthalene + Benzene System

REFERENCES

1. Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. *J. Chem. Eng. Data* 1985, *30*, 403-409.
2. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1959, 863-867.
3. Ward, H.L. *J. Phys. Chem.* 1926, *30*, 1316-1333.
4. Kravchenko, V.M. *Zhur. Fiz. Khim.* 1939, *13*, 133-145.
5. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
6. Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1964, *9*, 35-43.
7. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.7054	0.2946

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over metallic sodium distilled to a final purity of 99.95 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
310.35	0.6036	0.3964	334.35	0.3115	0.6885
315.55	0.5506	0.4494	344.15	0.1578	0.8422
323.45	0.4609	0.5391			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.708	0.292

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Spectroanalyzed, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
308.2	0.6234	0.3766	349.0	0.0820	0.9180
318.2	0.5194	0.4806			
320.6	0.4906	0.5094			
336.4	0.2881	0.7119			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
273.2	0.849	0.151
273.3	0.849	0.151
276.4	0.840	0.160
277.7	0.834	0.166
282.2	0.810	0.190
287.1	0.782	0.218
294.1	0.738	0.262
301.9	0.678	0.322
303.3	0.667	0.333
305.9	0.641	0.359
307.5	0.628	0.372
311.8	0.587	0.413
321.1	0.484	0.516
324.9	0.439	0.561
333.9	0.317	0.683
336.9	0.273	0.727
343.5	0.167	0.833

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gentle rotation to thoroughly mix contents. Bath temperature was slowly increased and solubility visually determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Purity not specified, synthesized by authors, recrystallized several times times until freezing point showed no further rise in temperature. Melting point temperature of sample was 5.5 °C.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

Zhur. Fiz. Khim. 1939, *13*, 133-145.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
276.5	0.969	0.031	(2)
274.3	0.934	0.066	(2)
273.2	0.919	0.081	(2)
272.2	0.905	0.095	(2)
270.7	0.880	0.120	(2)
269.6	0.866	0.134	Eutectic
269.7	0.859	0.141	(1)
277.2	0.831	0.169	(1)
283.8	0.793	0.207	(1)
290.4	0.752	0.248	(1)
296.2	0.711	0.289	(1)
301.7	0.668	0.332	(1)
307.4	0.620	0.380	(1)
312.8	0.572	0.428	(1)
317.7	0.524	0.476	(1)
322.2	0.469	0.531	(1)
327.2	0.411	0.589	(1)
331.4	0.352	0.648	(1)
335.4	0.289	0.711	(1)
340.2	0.224	0.776	(1)
344.2	0.155	0.845	(1)
349.7	0.079	0.921	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**EVALUATOR:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methylbenzene; C_7H_8; [108-88-3]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

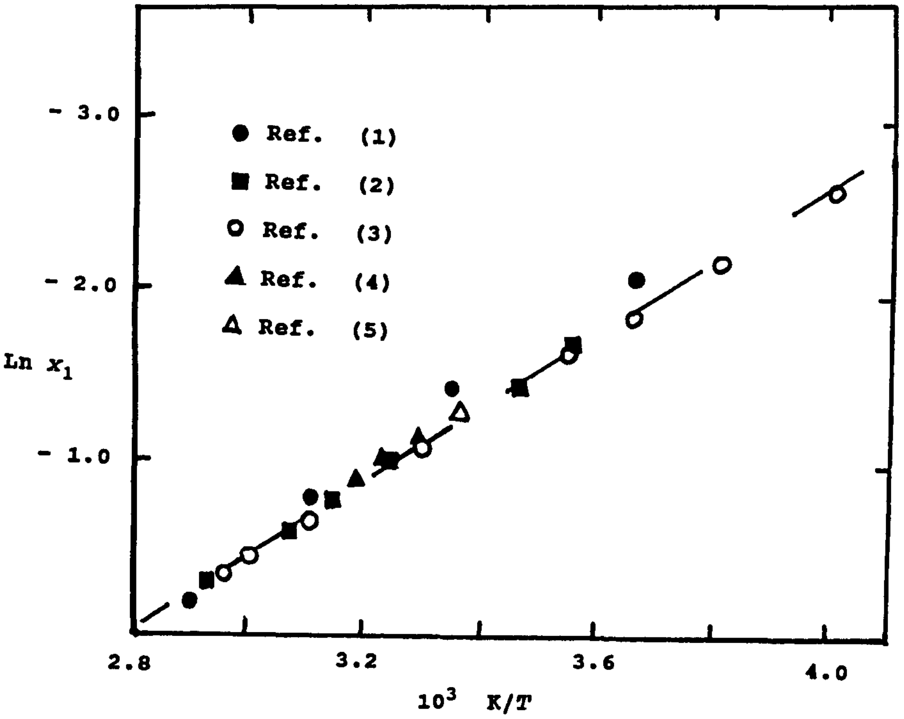
CRITICAL EVALUATION:

Naphthalene solubilities in methylbenzene were retrieved from papers by Speyers (1), Ward (2), Kravchenko (3), Acree *et al.* (4), Heric and Posey (5), and Chang (6). The first three studies report values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and both Heric and Posey and Chang measured the mole fraction solubility at the single temperature of 298 K. There is no a prior reason to exclude any of the six studies from the critical evaluation.

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

$$\text{Ln } x_1 = -1870.2\,(1/T) + 5.0916 \qquad (r = 0.9839)$$

for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Speyers, C.L. *Am. J. Sci.* 1902, *14*, 293-302.
2. Ward, H.L. *J. Phys. Chem.* 1926, *30*, 1316-1333.
3. Kravchenko, V.M. *Zhur. Fiz. Khim.* 1939, *13*, 133-145.
4. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
5. Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1964, *9*, 35-43.
6. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.7080	0.2920

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) ACS Grade, Matheson, Coleman and Bell, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.708	0.292

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
281.4	0.817	0.183	317.1	0.535	0.465
290.5	0.765	0.235	325.3	0.439	0.561
308.0	0.630	0.370	340.6	0.263	0.737

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Analyzed Grade, source not given, was fractionally distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Speyers, C.L.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
273.2	0.8718	0.1282	342.7	0.1557	0.8443
298.4	0.7674	0.2326			
319.5	0.5263	0.4737			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 80.1 °C.

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

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 8 % (relative error, compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methylbenzene; C_7H_8; [108-88-3]	Kravchenko, V.M. *Zhur. Fiz. Khim.* 1939, *13*, 133-145.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
177.7	0.988	0.012	(2)
177.2	0.978	0.022	Eutectic
188.2	0.975	0.025	(1)
200.7	0.971	0.029	(1)
214.2	0.963	0.037	(1)
217.7	0.956	0.044	(1)
227.1	0.948	0.052	(1)
246.6	0.925	0.075	(1)
261.9	0.887	0.113	(1)
273.0	0.845	0.155	(1)
281.2	0.806	0.194	(1)
289.1	0.763	0.237	(1)
296.2	0.720	0.280	(1)
303.2	0.675	0.325	(1)
307.5	0.628	0.372	(1)
313.4	0.587	0.413	(1)
317.7	0.531	0.469	(1)
321.4	0.483	0.517	(1)
331.2	0.373	0.627	(1)
338.2	0.256	0.744	(1)
346.4	0.121	0.879	(1)

Author reports eutectic point occurs at x_1 = 0.022 and T/K = 177.2.

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.* 1939, *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 distilled before use.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. 1986, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.6709	0.3291	40.0	0.5784	0.4216
35.0	0.6289	0.3711			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and gas chromatograph.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E.L.; Posey, C.D.

J. Chem. Eng. Data 1964, *9*, 35-43.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.7074	0.2926

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) ACS Grade, Matheson, Coleman and Bell, USA, was dried over calcium hydride and distilled to a final purity of 99.8 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:

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

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

EVALUATOR:

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

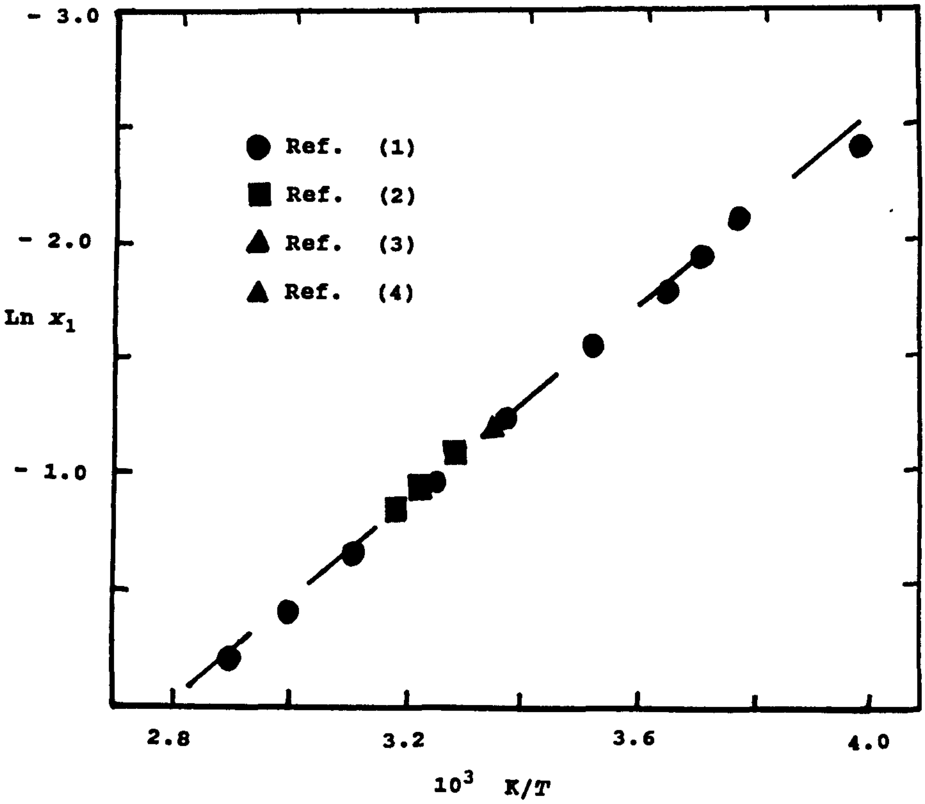
CRITICAL EVALUATION:

Naphthalene solubilities in ethylbenzene were retrieved from papers by Kravchenko (1), Acree *et al.* (2), Heric and Posey (3), and Chang (4). The first study reports values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and both Heric and Posey and Chang measured only the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the four studies from the critical evaluation.

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

$$\text{Ln } x_1 = -2162.0\ (1/T) + 6.0544 \qquad (r = 0.9979)$$

for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Kravchenko, V.M. *Zhur. Priklad. Khim.* 1949, *22*, 724-733.
2. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
3. Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1964, *9*, 35-43.
4. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethylbenzene; C_8H_{10}; [100-41-4]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.711	0.289

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethylbenzene; C_8H_{10}; [100-14-4]	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
VARIABLES:	**PREPARED BY:**
T/K = 303, 308 and 313	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.6712	0.3288	40.0	0.5767	0.4233
35.0	0.6295	0.3705			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and gas chromatograph.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethylbenzene; C_8H_{10}; [100-41-4]	Kravchenko, V.M. *Zhur. Priklad. Khim.* 1949, *22*, 724-733.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
178.8	1.000	0.0000	(2)
179.2	0.986	0.0142	(2)
178.2	0.983	0.0174	Eutectic
186.2	0.979	0.0210	(1)
203.2	0.974	0.0258	(1)
221.7	0.965	0.0351	(1)
241.7	0.939	0.0613	(1)
251.2	0.914	0.0860	(1)
265.2	0.881	0.119	(1)
270.7	0.860	0.140	(1)
274.7	0.837	0.163	(1)
283.4	0.793	0.207	(1)
296.2	0.713	0.287	(1)
307.2	0.623	0.377	(1)
320.7	0.489	0.511	(1)
332.2	0.331	0.669	(1)
343.7	0.168	0.832	(1)
353.2	0.000	1.000	(1)

Author reports eutectic occurs at x_1 = 0.0174 and at T/K = 178.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

Zhur. Priklad. Khim. 1949, *22*, 724-733.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
247.7	1.000	0.000	(2)
246.2	0.963	0.037	(2)
245.7	0.945	0.055	(2)
245.2	0.934	0.066	Eutectic
249.2	0.926	0.074	(1)
259.2	0.899	0.101	(1)
272.7	0.848	0.152	(1)
282.7	0.797	0.203	(1)
298.7	0.689	0.311	(1)
309.2	0.594	0.406	(1)
313.9	0.548	0.452	(1)
318.5	0.493	0.507	(1)
326.2	0.401	0.599	(1)
332.2	0.316	0.684	(1)
340.2	0.198	0.802	(1)
346.4	0.103	0.897	(1)
353.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]	Kravchenko, V.M. *Zhur. Fiz. Khim.* 1939, *13*, 989-1000.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
224.7	0.975	0.025	(2)
224.2	0.964	0.036	Eutectic
231.0	0.958	0.042	(1)
239.7	0.941	0.059	(1)
252.7	0.916	0.084	(1)
265.0	0.876	0.124	(1)
277.2	0.828	0.172	(1)
285.7	0.785	0.215	(1)
292.8	0.738	0.262	(1)
298.2	0.695	0.305	(1)
305.2	0.648	0.352	(1)
310.9	0.595	0.405	(1)
315.2	0.549	0.451	(1)
324.7	0.447	0.553	(1)
331.2	0.354	0.646	(1)
339.2	0.231	0.769	(1)
346.0	0.117	0.883	(1)

Author reporst eutectic point occurs at about x_1 = 0.036 and T/K = 224.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

Zhur. Priklad. Khim. 1949, *22*, 724-733.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
286.5	1.000	0.000	(2)
283.8	0.949	0.051	(2)
281.2	0.893	0.107	(2)
279.2	0.850	0.150	(2)
277.4	0.818	0.182	Eutectic
281.2	0.799	0.201	(1)
290.5	0.746	0.254	(1)
297.2	0.698	0.302	(1)
310.2	0.590	0.410	(1)
318.4	0.497	0.503	(1)
325.0	0.406	0.594	(1)
333.2	0.299	0.701	(1)
339.8	0.203	0.797	(1)
347.2	0.098	0.902	(1)
353.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Biphenyl; $C_{12}H_{10}$; [92-52-4]

ORIGINAL MEASUREMENTS:

Lee, H.H.; Warner, J.C.

J. Am. Chem. Soc. 1935, *57*, 318-321.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
342.2	1.000	0.000	(2)
336.7	0.898	0.102	(2)
331.0	0.806	0.194	(2)
323.5	0.700	0.300	(2)
321.0	0.657	0.343	(2)
316.1	0.600	0.400	(2)
315.7	0.573	0.427	(2)
313.0	0.556	0.444	(2)
312.8	0.555	0.445	
312.9	0.553	0.447	(1)
313.2	0.552	0.448	(1)
313.0	0.550	0.450	(1)
314.2	0.541	0.459	(1)
315.7	0.526	0.474	(1)
318.6	0.500	0.500	(1)
322.8	0.449	0.551	(1)
326.8	0.400	0.600	(1)
327.5	0.393	0.607	(1)
334.3	0.303	0.697	(1)
334.0	0.300	0.700	(1)
339.3	0.230	0.770	(1)
353.3	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Highest Purity, Eastman Chemicals, was recrystallized.

(2) Highest Purity, Eastman Chemicals, was recrystallized.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

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

(2) 1,2-Diphenylethane; $C_{14}H_{14}$; [103-29-7]

ORIGINAL MEASUREMENTS:

Lee, H.H.; Warner, J.C.

J. Am. Chem. Soc. 1935, *57*, 318-321.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
324.5	1.000	0.000	(2)
320.2	0.900	0.100	(2)
315.5	0.799	0.201	(2)
310.7	0.701	0.299	(2)
307.9	0.649	0.351	(2)
306.1	0.620	0.380	(2)
305.7	0.614	0.386	Eutectic
306.2	0.610	0.390	(1)
309.7	0.580	0.420	(1)
318.6	0.490	0.510	(1)
327.1	0.390	0.610	(1)
339.6	0.228	0.772	(1)
341.3	0.199	0.801	(1)
353.3	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.385 and *T*/K = 305.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Highest Purity, Eastman Chemicals, was recrystallized

(2) Highest Purity, Eastman Chemicals, was recrystallized.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.6	0.6365	0.3635	330.1	0.3728	0.6272
311.7	0.5859	0.4141			
318.4	0.5180	0.4820			
323.7	0.4494	0.5506			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.
(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

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

(2) 4-Isopropyl methylbenzene; $C_{10}H_{14}$; [99-87-6]

ORIGINAL MEASUREMENTS:

Wheeler, A.S.

J. Am. Chem. Soc. 1920, *42*, 1842-1846.

VARIABLES:

T/K = 303.2

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
30.0	0.8704	0.1296

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Indene; C_9H_8; [95-13-6]

ORIGINAL MEASUREMENTS:

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

J. Appl. Chem. U.S.S.R. 1952, *25*, 343-350. (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
271.4	271.4	1.000	0.000
272.2	271.7	0.964	0.036
273.2	272.2	0.951	0.049
278.2	275.2	0.907	0.093
282.4	277.2	0.870	0.130
288.2	282.2	0.820	0.180
290.3	283.2	0.799	0.201
297.0	290.2	0.739	0.261
298.7	291.2	0.720	0.280
307.7	300.2	0.625	0.375
316.7	307.2	0.540	0.460
317.2	308.2	0.530	0.470
326.3	316.2	0.426	0.574
326.4	317.2	0.423	0.577
332.5	325.2	0.332	0.668
339.7	326.2	0.228	0.772
353.2	353.2	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a complete series of solid solutions. Melting points of binary mixtures lie between those of the two pure components. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Fluoranthene; $C_{16}H_{10}$; [206-44-0]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
383.2	1.000	0.000	(2)
374.2	0.875	0.125	(2)
361.4	0.707	0.293	(2)
352.8	0.614	0.386	(2)
343.5	0.519	0.471	(2)
337.1	0.461	0.539	(2)
330.9	0.411	0.589	(2)
329.0	0.390	0.610	Eutectic
332.2	0.337	0.663	(1)
338.5	0.247	0.753	(1)
346.3	0.117	0.883	(1)
353.4	0.000	1.000	(1)

Authors report eutectic point occurs at x_2 = 0.390 and at T/K = 329.0.

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.* 1939, *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:

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

(2) Fluorene; $C_{13}H_{10}$; [86-73-7]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

J. Appl. Chem. U.S.S.R. 1952, *25*, 1015-1022. (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
387.2	1.000	0.000	(2)
377.6	0.879	0.121	(2)
368.5	0.753	0.247	(2)
358.6	0.641	0.359	(2)
348.7	0.534	0.466	(2)
337.0	0.436	0.564	(2)
329.7	0.388	0.612	(2)
328.2	0.375	0.625	(2)
329.4	0.342	0.658	(1)
335.7	0.245	0.755	(1)
342.4	0.156	0.844	(1)
347.5	0.079	0.921	(1)
353.2	0.000	1.000	(1)

Author reports eutectic point occurs at x_1 = 0.635 and at T/K = 328.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Chrysene; $C_{18}H_{12}$; [218-01-9]	Kravchenko, V.M.; Pastukhova, I.S. *Proc. Acad. Sci. U.S.S.R., Sect. Chem.* 1956, *111*, 667-669. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
528.2	1.000	0.000	(2)
520.2	0.903	0.097	(2)
511.4	0.817	0.183	(2)
500.2	0.702	0.298	(2)
487.5	0.593	0.407	(2)
476.2	0.504	0.496	(2)
459.7	0.407	0.593	(2)
442.4	0.290	0.710	(2)
417.8	0.202	0.798	(2)
406.2	0.157	0.843	(2)
388.4	0.103	0.897	(2)
351.0	0.042	0.958	Eutectic
351.7	0.025	0.975	(1)
353.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Pyrene; $C_{16}H_{10}$; [129-00-0]

ORIGINAL MEASUREMENTS:

Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M.
Bull. Chem. Soc. Japan 1985, *58*, 3643-3644.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the original paper, shows that the system is a simple eutectic system. The eutectic point occurs at circa x_2 = 0.22 and T/K = 335.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical grade, Katayama Chemicals, Japan, was used as received.

(2) Reagent grade, Katayama Chemicals, Japan, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.02 (Compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

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

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Furfuryl Acetate; $C_7H_8O_3$; [623-17-6]	**ORIGINAL MEASUREMENTS:** Sunier, A.A. *J. Phys. Chem.* 1931, *35*, 1756-1761.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
292.6	0.804	0.196
310.6	0.659	0.341
314.1	0.622	0.378
319.4	0.562	0.438
321.5	0.534	0.466
321.5	0.528	0.472
329.4	0.416	0.584
334.6	0.338	0.662
338.4	0.271	0.729
343.2	0.184	0.816

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.
(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methyl 2-furoate; $C_6H_6O_3$; [611-13-2]	**ORIGINAL MEASUREMENTS:** Sunier, A.A. *J. Phys. Chem.* 1931, *35*, 1756-1761.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.9	0.7516	0.2484	330.0	0.408	0.592
308.2	0.687	0.313	341.1	0.220	0.780
315.5	0.608	0.392			
325.0	0.484	0.516			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.
(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethyl 2-furoate; $C_7H_8O_3$; [614-99-3]	**ORIGINAL MEASUREMENTS:** Sunier, A.A. *J. Phys. Chem.* 1931, *35*, 1756-1761.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
298.8	0.712	0.288	336.7	0.277	0.723
307.0	0.647	0.353	340.0	0.224	0.776
318.1	0.530	0.470			
328.7	0.396	0.604			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.
(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) n-Propyl 2-furoate; $C_8H_{10}O_3$; [615-10-1]

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1931, *35*, 1756-1761.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
298.8	0.697	0.303	333.1	0.326	0.674
309.6	0.607	0.393	341.1	0.108	0.791
318.5	0.519	0.481			
323.4	0.456	0.544			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) n-Butyl 2-furoate; $C_9H_{12}O_3$; [583-33-5]

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1931, *35*, 1756-1761.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
294.5	0.768	0.232	328.1	0.385	0.615
307.1	0.617	0.383	338.1	0.246	0.754
312.4	0.566	0.434			
320.9	0.477	0.523			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) 1,1-Oxybisethane; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2^a	x_1^a
25.0	0.753	0.247

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

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

Bennett, G.M.; Philip, W.G.

J. Chem. Soc. 1928, 1937-1942.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
315.8	0.6227	0.3773
318.9	0.5847	0.4153
326.1	0.4922	0.5078

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

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

(2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: 0.0001. (compiler).

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Ethoxypropane; $C_5H_{12}O$; [628-32-0]	**ORIGINAL MEASUREMENTS:** Bennett, G.M.; Philip, W.G. *J. Chem. Soc.* 1928, 1937-1942.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
303.1	0.7292	0.2708
312.9	0.6350	0.3650
315.5	0.6064	0.3936

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

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

(2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: 0.0001. (compiler).

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2-Ethoxypropane; $C_5H_{12}O$; [625-54-7]	**ORIGINAL MEASUREMENTS:** Bennett, G.M.; Philip, W.G. *J. Chem. Soc.* 1928, 1937-1942.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
317.1	0.5974	0.4026
325.5	0.4864	0.5136

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

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

(2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: 0.0001. (compiler).

COMPONENTS:

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

(2) 2,2-Dimethyloxetane; $C_5H_{10}O$;
[6245-99-4]

ORIGINAL MEASUREMENTS:

Bennett, G.M.; Philip, W.G.

J. Chem. Soc. 1928, 1937-1942.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
307.0	0.6990	0.3010
313.1	0.5913	0.4087
317.9	0.5443	0.4557

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

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

(2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: 0.0001. (compiler).

COMPONENTS:

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

(2) 3,3-Dimethyloxetane; $C_5H_{10}O$;
[6921-35-3]

ORIGINAL MEASUREMENTS:

Bennett, G.M.; Philip, W.G.

J. Chem. Soc. 1928, 1937-1942.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
302.4	0.6540	0.3460
312.1	0.5827	0.4173

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

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

(2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: 0.0001. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrahydropyran; $C_5H_{10}O$; [142-68-7]	Bennett, G.M.; Philip, W.G. *J. Chem. Soc.* 1928, 1937-1942.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
299.6	0.6579	0.3421
303.3	0.6295	0.3705
313.4	0.5392	0.4608

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

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

(2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: 0.0001. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Dichloromethane; CH_2Cl_2; [75-09-2]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.670	0.330

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, J. T. Baker Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.661	0.339

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	Mahieu, J. *Bull. Soc. Chim. Belgique* 1936, *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	0.660	0.340

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

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	Speyers, C.L. *Am. J. Sci.* 1902, *14*, 293-302.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
273.0	0.8042	0.1958
283.8	0.7686	0.2314
303.5	0.6147	0.3853
325.7	0.4260	0.5740

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 80.1 °C.

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1964, *9*, 35-43.
VARIABLES:	**PREPARED BY:**
$T/K = 298$	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.7409	0.2591

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision refractometer.

Excess solute and solvent placed in glass bottles and allowed to equilibrate with gentle agitation for several days at constant temperature. Refractive indices of saturated solutions were measured and solubilities obtained using a calibration curve. Attainment of equilibrium verified by making repetitive measurements after several additional days.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.

(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: precision ± 0.0005.

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

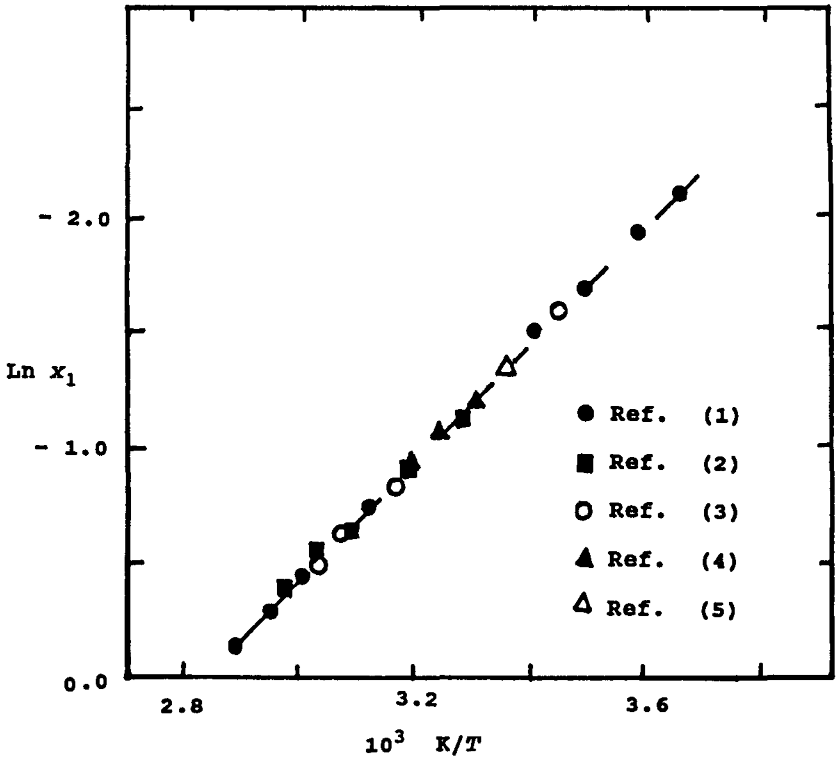
CRITICAL EVALUATION:

Naphthalene solubilities in tetrachloromethane were retrieved from papers by Ward (1), McLaughlin and Zainal (2), Heric and Yeh (3), Acree *et al.* (4), Heric and Posey (5) and Chang (6). The first three studies report values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and both Heric and Posey and Chang measured the mole fraction solubility at the single temperature of 298 K. There is no a prior reason to exclude any of the six studies from the critical evaluation.

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

$$\text{Ln } x_1 = -2626.1\,(1/T) + 7.4567 \qquad (r = 0.9999)$$

for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Ward, H.L. *J. Phys. Chem.* 1926, *30*, 1316-1333.
2. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 2485-2488.
3. Heric, E.L.; Yeh, K.-N. *J. Chem. Eng. Data* 1970, *15*, 13-17.
4. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
5. Heric, E.L.; Posey, C.D. *J. Chem. Eng. Data* 1964, *9*, 35-43.
6. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Heric, E. L; Yeh, K.-N.

J. Chem. Eng. Data 1970, *15*, 13-17.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
286.64	0.8188	0.1812	323.84	0.4731	0.5269
290.51	0.7961	0.2039	328.58	0.4085	0.5915
300.17	0.7262	0.2738	334.92	0.3120	0.6880
316.25	0.5671	0.4329	342.33	0.1935	0.8065

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, Baker Chemical Company, USA, was used as received.

(2) Reagent Grade, Baker Chemical Company, was stored over phosphorous pentoxide and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.03.
x_1: ± 0.0001.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.745	0.255

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.6	0.880	0.120	312.7	0.611	0.389
279.2	0.857	0.143	320.1	0.525	0.475
286.2	0.822	0.178	331.5	0.369	0.631
292.7	0.783	0.217	338.0	0.269	0.731
301.4	0.718	0.282	345.6	0.142	0.858

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Purity and source not specified, was fractionally distilled twice, collecting fraction at 76.70-76.75 °C.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

(1) Naphthalene; $C_{10}H$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
304.8	0.6871	0.3129	336.0	0.3008	0.6992
314.2	0.5954	0.4046			
322.8	0.4868	0.5132			
329.2	0.3990	0.6010			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
VARIABLES:	**PREPARED BY:**
T/K = 303, 308 and 313	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.6988	0.3012	40.0	0.6019	0.3981
35.0	0.6538	0.3462			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and gas chromatograph.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Trichloroethylene; C_2HCl_3; [79-01-6]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639-646.
VARIABLES:	**PREPARED BY:**
T/K = 296	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	3.46

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C_8H_{10}; [91-20-3] (2) Diiodomethane; CH_2I_2; [75-11-6]	Domanska, U. *Polish J. Chem.* 1981, *55*, 1715-1720. (numerical values obtained through personal communication with author.)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
321.85	0.5619	0.4381	295.85	0.8407	0.1593
319.10	0.6033	0.3967	291.00	0.8690	0.1310
313.00	0.6858	0.3142	286.55	0.8906	0.1094
307.00	0.7515	0.2485	281.75	0.9096	0.0904
301.85	0.7983	0.2017			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Chemapol, Czech., was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,1-Dibromoethane; $C_2H_4Br_2$; [557-91-5]	Sunier, A.A.; Rosenblum, C. *J. Phys. Chem.* 1928, *32*, 1047-1055.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
297.1	0.685	0.315	336.2	0.274	0.726
317.3	0.504	0.496	341.7	0.193	0.807
321.6	0.455	0.545	347.5	0.102	0.898
326.9	0.396	0.606			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,2-Dibromoethane; $C_2H_4Br_2$; [106-93-4]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.697	0.303

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,2-Dibromoethane; $C_2H_4Br_2$; [106-93-4]	Sunier, A.A.; Rosenblum, C. *J. Phys. Chem.* 1928, *32*, 1047-1055.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
293.9	0.732	0.268	334.9	0.295	0.705
308.5	0.608	0.392	342.1	0.190	0.810
317.6	0.515	0.485	350.0	0.054	0.946
328.3	0.386	0.616			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 1,1-Dichloroethane; $C_2H_4Cl_2$; [75-34-3]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.691	0.309

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

(2) 1,1-Dichloroethane; $C_2H_4Cl_2$; [75-34-3]

ORIGINAL MEASUREMENTS:

Sunier, A.A.; Rosenblum, C.

J. Phys. Chem. 1928, *32*, 1047-1055.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.2	0.626	0.374	335.8	0.290	0.710
316.5	0.530	0.470	343.0	0.176	0.824
324.0	0.445	0.555	348.8	0.081	0.919
331.8	0.346	0.654			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.
(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{o}C$	x_2	x_1
25.0	0.680	0.320

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

(2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

ORIGINAL MEASUREMENTS:

Sunier, A.A.; Rosenblum, C.

J. Phys. Chem. 1928, *32*, 1047-1055.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.4	0.664	0.336	332.6	0.322	0.678
309.7	0.581	0.419	342.9	0.173	0.827
319.3	0.485	0.515	348.9	0.082	0.918
324.3	0.428	0.572			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.689	0.311

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 visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.	(1) Purity, source and purification procedures not specified. (2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received. **ESTIMATED ERRORS:** T/K: precision ± 0.1. x_1: ± 2 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Ward, H.L. *J. Phys. Chem.* <u>1926</u>, *30*, 1316-1333.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
277.4	0.815	0.185	316.0	0.527	0.473
282.0	0.792	0.208	322.2	0.460	0.540
295.3	0.708	0.292	335.8	0.284	0.716
302.6	0.651	0.349			

AUXILIARY INFORMATION

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 visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.	(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C. (2) Purity and commercial supplier not given, was fractionally distilled three times through a Hempel column. **ESTIMATED ERRORS:** T/K: precision ± 0.1. x_1: to 3 significant figs. (compiler).

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]	**ORIGINAL MEASUREMENTS:** Morris, R.E.; Cook, W.A. *J. Am. Chem. Soc.* 1935, *57*, 2403-2406.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
326.4	1.000	0.000	(2)
323.7	0.950	0.050	(2)
319.6	0.881	0.119	(2)
313.3	0.771	0.229	(2)
308.8	0.699	0.301	(2)
305.0	0.652	0.348	(2)
304.3	0.639	0.361	(2)
304.1	0.632	0.368	(2)
303.4	0.606	0.396	
304.8	0.591	0.409	(1)
311.7	0.531	0.469	(1)
316.5	0.490	0.510	(1)
320.5	0.447	0.553	(1)
326.6	0.378	0.622	(1)
332.9	0.308	0.692	(1)
342.1	0.182	0.818	(1)
347.0	0.106	0.894	(1)
353.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified, was purified by distillation.

(2) Purity and chemical source were not specified, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

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

(2) Hexafluorobenzene; C_6F_6; [392-56-3]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Messer, C.E.

J. Chem. Soc., Sect. A 1966, 1106-1110.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
346.80	0.1177	0.8823
348.30	0.0895	0.9105
349.80	0.0647	0.9353
351.75	0.0293	0.9707

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Molecular Weight Grade, Hopkin and Williams, was passed over an alumina column, recrystallized and sublimed.

(2) Purity not given, Imperial Smelting, Ltd., Avonmouth, Bristol, was dried over anhydrous calcium sulfate.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Octafluoronaphthalene; $C_{10}F_8$; [313-72-4]

ORIGINAL MEASUREMENTS:

Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M.
Bull. Chem. Soc. Japan 1985, *58*, 3643-3644.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the original paper, shows formation of a 1:1 naphthalene - octafluoronaphthalene molecular compound having a melting point of circa 408.2 K. Two eutectic points occur at about x_2 = 0.09 and T/K = 350.2, and at about x_2 = 0.88 and T/K = 358.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical grade, Katayama Chemicals, Japan, was used as received.

(2) Reagent grade, Tokyo Chemical Company, Japan, was recrystallized from methanol before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.02 (Compiler).

COMPONENTS:	**EVALUATOR:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methanol; CH_4O; [67-56-1]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

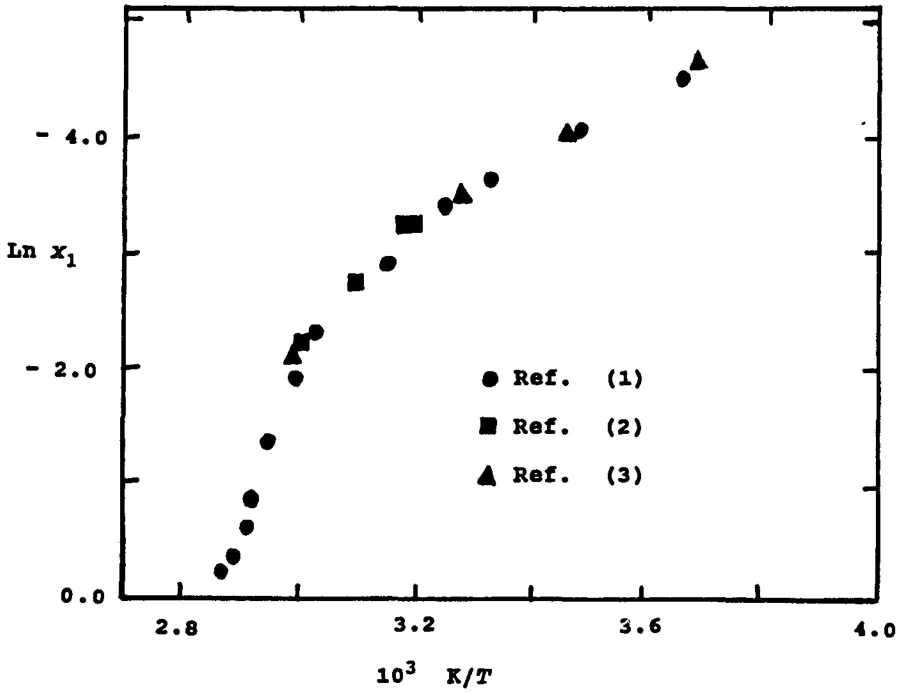
CRITICAL EVALUATION:

Naphthalene solubilities in methanol were retrieved from papers by Ward (1), Sunier (2), Speyers (3), Dickhut *et al.* (4) and Pinal *et al.* (5). The first three studies report values at several temperatures, whereas Dickhut *et al.* and Pinal *et al.* measured only the mole fraction solubility at a single temperature of 298 K and 296 K, respectively. There is no a prior reason to exclude any of the five studies from the critical evaluation.

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

$$\text{Ln } x_1 = -5574.0\,(1/T) + 14.998 \qquad (r = 0.9280)$$

for variation of naphthalene solubility with absolute temperature (see graph below). Nonlinear behavior indicates a nonconstant enthalpy of solution, probably caused by self-associating hydrogen-bonding character of methanol.



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Ward, H.L. *J. Phys. Chem.* 1926, *30*, 1316-1333.
2. Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
3. Speyers, C.L. *Am. J. Sci.* 1902, *14*, 293-302.
4. Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. *J. Chem. Eng. Data* 1989, *34*, 438-443.
5. Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639-646.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
274.0	0.989	0.0107
286.7	0.984	0.0163
299.5	0.974	0.0255
306.8	0.967	0.0333
310.6	0.961	0.0390
317.1	0.948	0.052
329.9	0.898	0.102
334.0	0.857	0.143
338.9	0.745	0.255
341.6	0.613	0.387
342.7	0.503	0.497
344.9	0.334	0.666
346.0	0.268	0.732
347.1	0.206	0.794
347.5	0.180	0.820

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gentle rotation to thoroughly mix contents. Bath temperature was slowly increased and solubility visually determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Absolute, commercial supplier not identified, fractionally distilled over sodium metal, collecting the fraction at 64.7-64.8 °C.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.1.

x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1930, *34*, 2582-2597.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
313.4	0.9610	0.0390	341.8	0.6093	0.3907
322.1	0.9412	0.0588			
331.6	0.8980	0.1020			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) C.P. Grade, source not given, was refluxed over lime once and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0002. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1930, *34*, 2582-2597.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
310.8	0.9626	0.0374	313.3	0.9583	0.0417
321.0	0.9413	0.0587	320.8	0.9418	0.0582
331.1	0.8938	0.1062	330.6	0.8976	0.1024

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) C.P. Grade, source not given, was refluxed over lime twice and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0002. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data <u>1989</u>, *34*, 438-443.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9765	0.0235

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solution were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.9 %, source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.05 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. <u>1990</u>, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
23.0	0.616

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Speyers, C.L.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9913	0.0087	321.2	0.9417	0.0583
287.8	0.9832	0.0168	333.1	0.8766	0.1234
305.0	0.9703	0.0297			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 80.1 °C.

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Speyers, C.L.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9820	0.0180	320.1	0.9030	0.0970
281.8	0.9787	0.0213	343.0	0.3577	0.6423
305.0	0.9518	0.0482			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 80.1 °C.

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

ESTIMATED ERRORS:

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

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

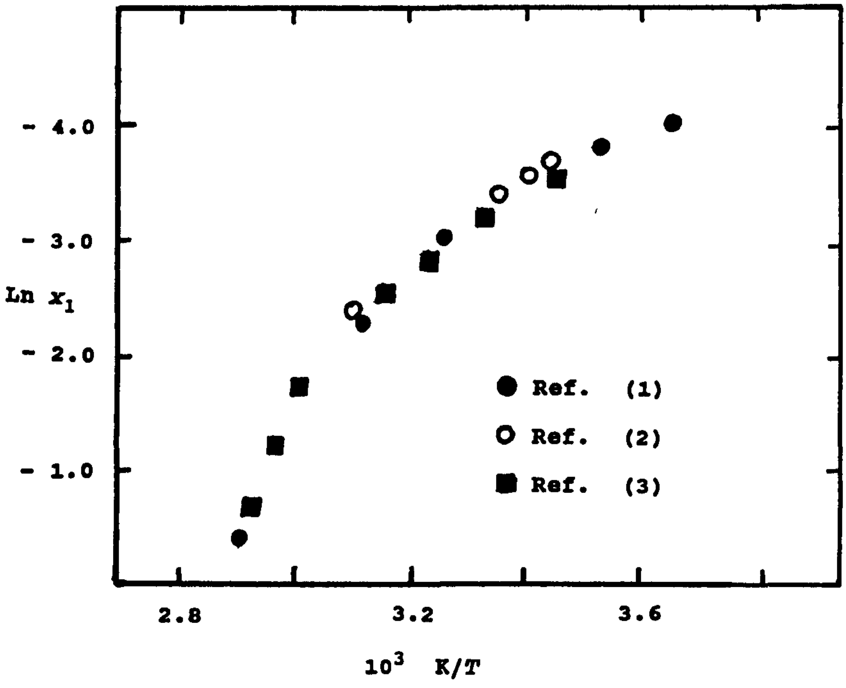
CRITICAL EVALUATION:

Naphthalene solubilities in ethanol were retrieved from papers by Speyers (1), Domanska (2), Sunier (3) and Dickhut *et al.* (4). The first three studies report values at several temperatures, whereas Dickhut *et al.* (4) measured only the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the four studies from the critical evaluation.

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

$$\text{Ln}\ x_1 = -4761.8\ (1/T) + 12.740 \qquad (r = 0.9461)$$

for variation of naphthalene solubility with absolute temperature (see graph below). Nonlinear behavior indicates a nonconstant enthalpy of solution, probably caused by self-associating hydrogen-bonding character of ethanol.



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Speyers, C.L. *Am. J. Sci.* 1902, *14*, 293-302.
2. Domanska, U. *Polish J. Chem.* 1981, *55*, 1715-1720.
3. Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
4. Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. *J. Chem. Eng. Data* 1989, *34*, 438-443.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5]	Domanska, U. *Polish J. Chem.* 1981, *55*, 1715-1720. (numerical values obtained through personal correspondence with author.)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
290.50	0.976	0.024	305.65	0.958	0.042
294.30	0.972	0.028	308.80	0.952	0.048
298.15	0.968	0.032	322.20	0.913	0.087
302.20	0.963	0.037			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations were sealed in ampoules and placed in constant temperature to equilibrate. Bath temperature was slowly increased. Solubility determined by visually noting temperature at which last trace of solid disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.
(2) Initial purity not specified, Reachim., Poland, was dried over phosphorous pentoxide and fractionally distilled to a final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5]	Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
288.9	0.9708	0.0292	320.2	0.9000	0.1000
299.0	0.9578	0.0422	330.3	0.8184	0.1816
308.4	0.9405	0.0595	336.2	0.7006	0.2994
316.3	0.9171	0.0829	340.9	0.5035	0.4965

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.
(2) 95 %, source not specified, was refluxed over lime and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data <u>1989</u>, *34*, 438-443.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9602	0.0398

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solution were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 200 Proof, source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.05 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. <u>1930</u>, *34*, 2582-2597.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
296.1	0.9524	0.0476	323.0	0.8491	0.1509
301.1	0.9429	0.0571	327.0	0.8074	0.1926
309.2	0.9208	0.0792	332.5	0.7209	0.2791
310.4	0.9168	0.0832	340.1	0.4751	0.5249
314.9	0.8983	0.1017	342.7	0.3495	0.6505

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

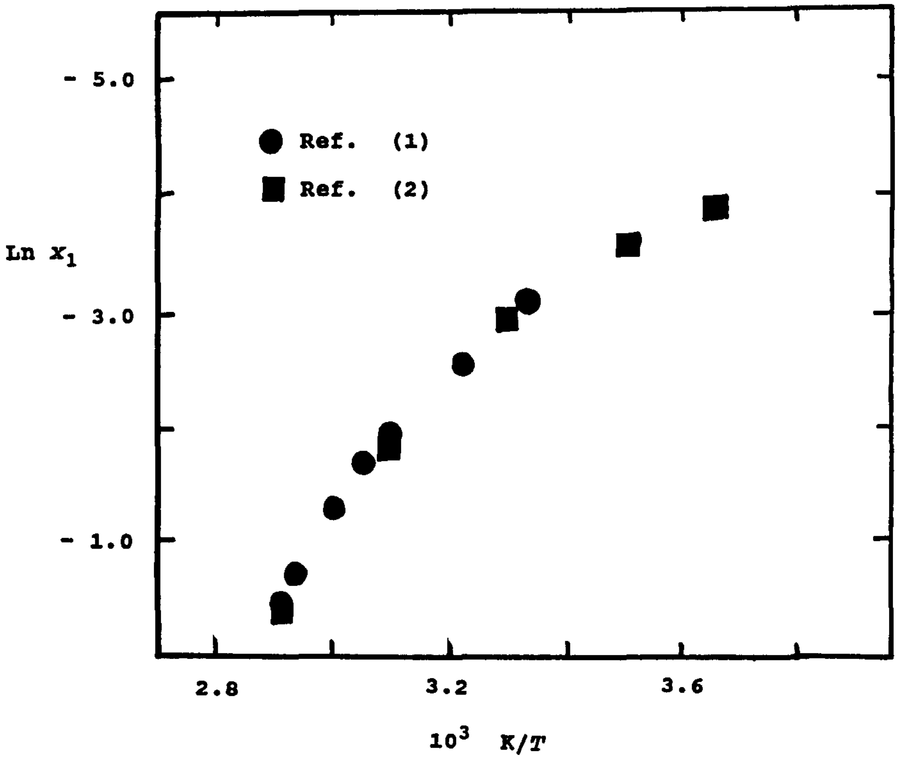
CRITICAL EVALUATION:

Naphthalene solubilities in 1-propanol were retrieved from papers by Sunier (1), Speyers (2) and Dickhut *et al.* (3). The first two studies report observed values at several temperatures, whereas Dickhut *et al.* determined only a single mole fraction solubility for 298 K. There is no a prior reason to exclude any of the three studies from the critical evaluation.

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

$$\text{Ln } x_1 = -4803.1\,(1/T) + 13.193 \qquad (r = 0.9694)$$

for variation of naphthalene solubility with absolute temperature (see graph below). Nonlinear behavior indicates a nonconstant enthalpy of solution, probably caused by self-associating hydrogen-bonding character of 1-propanol.



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
2. Speyers, C.L. *Am. J. Sci.* 1902, *14*, 293-302.
3. Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. *J. Chem. Eng. Data* 1989, *34*, 438-443.

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9495	0.0505

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solution were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.5 %, source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.05 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Speyers, C.L.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9791	0.0209	323.5	0.8466	0.1534
283.6	0.9730	0.0270	341.7	0.3710	0.6290
303.5	0.9466	0.0534			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 80.1 °C.

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

ESTIMATED ERRORS:

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

COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2-Propanol; C_3H_8O; [67-63-0]	**ORIGINAL MEASUREMENTS:** Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
297.6	0.9629	0.0371
304.1	0.9508	0.0492
308.5	0.9392	0.0608
311.0	0.9312	0.0688
316.0	0.9115	0.0885
318.4	0.8988	0.1012
324.9	0.8503	0.1497
328.1	0.8122	0.1878
333.4	0.7124	0.2876
339.0	0.5227	0.4773
343.1	0.3295	0.6705

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was stored over lime and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

EVALUATOR:

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

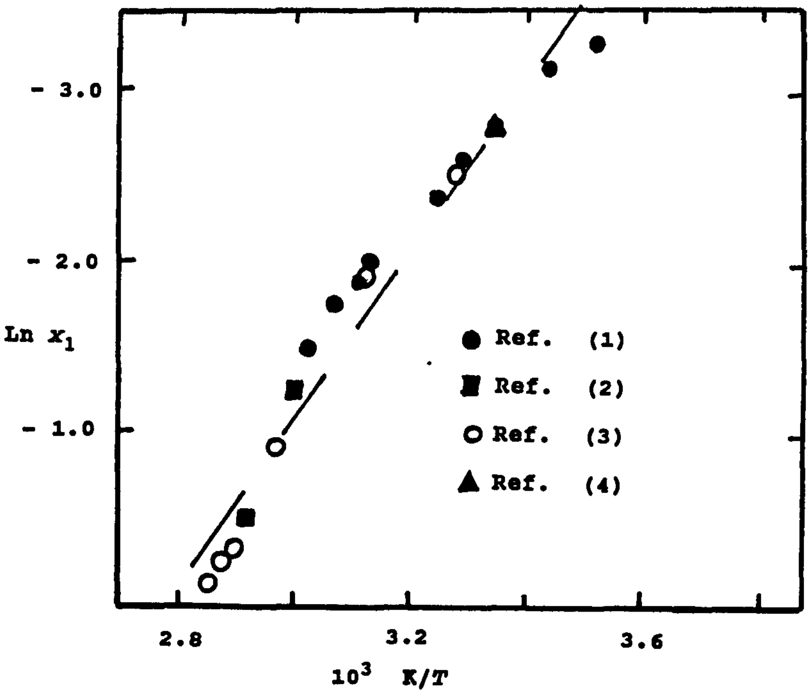
CRITICAL EVALUATION:

Naphthalene solubilities in 1-butanol were retrieved from papers by Domanska (1), Sunier (2), Ward (3) and Dickhut *et al.* (4). The first three studies report values at several temperatures, whereas Dickhut *et al.* (4) measured only the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the four studies from the critical evaluation.

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

$$\text{Ln } x_1 = -4963.6\ (1/T) + 13.865 \qquad (r = 0.9814)$$

for variation of naphthalene solubility with absolute temperature (see graph below). Nonlinear behavior indicates a nonconstant enthalpy of solution, probably caused by self-associating hydrogen-bonding character of 1-butanol.



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Domanska, U. *Polish J. Chem.* 1981, *55*, 1715-1720.
2. Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
3. Ward, H.L. *J. Phys. Chem.* 1926, *30*, 1316-1333.
4. Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. *J. Chem. Eng. Data* 1989, *34*, 438-443.

COMPONENTS:

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

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Domanska, U.

Polish J. Chem. 1981, *55*, 1715-1720.
(numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
284.05	0.962	0.038
289.05	0.955	0.045
291.95	0.950	0.050
295.35	0.942	0.058
298.25	0.934	0.066
303.25	0.923	0.077
307.95	0.909	0.091
313.45	0.887	0.113
317.35	0.860	0.140
319.75	0.844	0.156
323.55	0.824	0.176
330.45	0.772	0.228

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, P.O.Ch., was dried over sodium carbonate and fractionally distilled to a final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
295.2	0.942	0.058
297.5	0.938	0.062
304.8	0.918	0.082
308.8	0.905	0.095
319.7	0.842	0.158
325.5	0.789	0.211
330.1	0.724	0.276
336.4	0.568	0.432
341.3	0.391	0.609
343.3	0.300	0.700
344.9	0.238	0.762
347.1	0.163	0.837
349.2	0.095	0.905

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gentle rotation to thoroughly mix contents. Bath temperature was slowly increased and solubility visually determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Purity not specified, from fermentation processes, fractionally distilled four times, collecting the last fraction at 117.6-117.8 °C.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	Sunier, A.A. *J. Phys. Chem.* 1930, *34*, 2582-2597.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.9	0.9061	0.0939	341.6	0.3745	0.6255
320.8	0.8348	0.1652			
331.0	0.7063	0.2937			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.
(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. *J. Chem. Eng. Data* 1989, *34*, 438-443.
VARIABLES: T/K = 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9334	0.0666

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solution were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99.9 %, source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.05 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

(2) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1930, *34*, 2582-2597.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.9	0.9344	0.0656	319.6	0.8381	0.1619
308.1	0.9116	0.0884	330.5	0.6757	0.3243
313.7	0.8830	0.1170	333.8	0.5952	0.4048
318.6	0.8477	0.1523	342.0	0.3894	0.6106

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1930, *34*, 2582-2597.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
292.7	0.9620	0.0380	323.6	0.8392	0.1608
309.5	0.9220	0.0780	333.5	0.6779	0.3221
310.8	0.9174	0.0826	336.3	0.5946	0.4054
314.1	0.9036	0.0964	343.4	0.2908	0.7092
322.8	0.8471	0.1529			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was stored over lime and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1930, *34*, 2582-2597.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
295.3	0.9614	0.0386	323.4	0.8181	0.1819
304.8	0.9348	0.0652	331.0	0.6910	0.3090
311.0	0.9107	0.0893	335.6	0.5630	0.4370
314.9	0.8896	0.1104	339.8	0.4604	0.5396
320.5	0.8483	0.1517			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0002. (compiler).

COMPONENTS:

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

(2) 1-Pentanol; $C_5H_{10}O$; [71-41-0]

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, *34*, 438-443.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9189	0.0811

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.

Excess solute and solvent placed in closed glass bottles, mixed at room temperature for 24 hours on magnetic stirrers and temperature equilibrated for an additional 24 hours in a constant temperature water bath. After equilibrium was obtained aliquots of saturated solution were removed and diluted quantitatively for spectrophotometric analysis at 254 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Scintillation grade, 99 %, source not given.

(2) 99 %, source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.05 (compiler).

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

COMPONENTS:

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

(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

ORIGINAL MEASUREMENTS:

Domanska, U.

Polish J. Chem., 1981, *55*, 1715-1720.
(numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
282.30	0.946	0.054
286.35	0.936	0.062
290.35	0.927	0.073
296.05	0.914	0.086
299.95	0.899	0.101
305.75	0.880	0.120
310.85	0.853	0.147
314.95	0.825	0.175
318.95	0.799	0.201
321.45	0.776	0.224
331.55	0.632	0.368

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Reachim, Poland, was dried over sodium carbonate and fractionally distilled to a final purity of 99.9+ %.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Domanska, U.

Polish J. Chem., 1981, *55*, 1715-1720.
(numerical values obtained through personal correspondence with author.)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
280.95	0.931	0.069
284.35	0.923	0.077
286.75	0.916	0.084
289.95	0.908	0.092
291.95	0.901	0.099
294.15	0.892	0.108
295.55	0.884	0.116
298.55	0.976	0.124
302.35	0.861	0.139
305.15	0.847	0.153
308.25	0.831	0.169
311.95	0.806	0.194
315.45	0.779	0.221
317.45	0.760	0.240
320.65	0.733	0.267
323.35	0.701	0.299
325.95	0.672	0.328
331.55	0.578	0.422

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass ampoules and placed in a constant temperature to equilibrate. Bath temperature was slowly increased by 2 K per hour. Solubility determined by visually noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, P.O.Ch., Gliwice, Poland, was vacuum sublimed to a melting temperature of 80.25 °C.

(2) Initial purity not specified, Koch-, Light, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.9589

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Cyclohexanol; $C_6H_{12}O$; [108-93-0]

ORIGINAL MEASUREMENTS:

Weissenberger, G.

Z. Angew Chem. 1927, *40*, 776.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
283	0.960	0.040	313	0.768	0.232
293	0.906	0.094	323	0.700	0.300
303	0.842	0.158			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental details were not given in paper.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.5. (compiler)
x_1: 0.002. (compiler).

COMPONENTS:

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

(2) Methylcyclohexanol; $C_7H_{14}O$; [25639-42-3]

ORIGINAL MEASUREMENTS:

Weissenberger, G.

Z. Angew Chem. <u>1927</u>, *40*, 776.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
283	0.965	0.035	313	0.767	0.233
293	0.921	0.079	318	0.616	0.384
303	0.861	0.139			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental details were not given in paper.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.5. (compiler)
x_1: 0.002. (compiler).

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [99-65-0]

(2) 1,4-Benzenediol; $C_6H_6O_2$; [123-31-9]

ORIGINAL MEASUREMENTS:

Kremann, R.; Janetzky, E.

Monatsch. Chem. <u>1911</u>, *32*, 1055-1062.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
445.2	1.000	0.000	423.2	0.225	0.775
432.2	0.913	0.087	412.1	0.115	0.885
429.2	0.823	0.177	403.2	0.092	0.908
428.2	0.636	0.364	383.2	0.038	0.962
427.4	0.538	0.462	361.2	0.015	0.985
426.2	0.375	0.625	353.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given.

(2) Purity and chemical source not given

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 1,2-Benzenediol; $C_6H_6O_2$; [120-80-9]

ORIGINAL MEASUREMENTS:

Kremann, R.; Janetzky, E.

Monatsch. Chem. 1911, *32*, 1055-1062.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
377.2	1.000	0.000
370.7	0.908	0.092
368.7	0.843	0.157
364.7	0.756	0.244
361.2	0.689	0.311
358.2	0.592	0.408
357.7	0.552	0.448
356.7	0.503	0.497
356.2	0.467	0.533
356.2	0.422	0.578
355.2	0.399	0.601
354.7	0.361	0.639
353.2	0.333	0.667
349.2	0.260	0.740
346.2	0.195	0.805
351.2	0.049	0.951
353.2	0.000	1.000

Compiler: A 1:1 molecular compound is probably formed, in which case the second eutectic point occurs at about x_1 = 0.815 and T/K = 345.6.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,3-Benzenediol; $C_6H_6O_2$; [108-46-3]	Kremann, R.; Janetzky, E. *Monatsch. Chem.* 1911, *32*, 1055-1062.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Phases
383.2	1.000	0.000	(2)
378.7	0.938	0.062	(2) + liq 1
375.2	0.896	0.104	(2) + liq 1
373.2	0.882	0.118	(2) + liq 1
373.7	0.839	0.161	(2) + liq 1
370.7	0.830	0.170	liq 1 + liq 2
374.7	0.823	0.177	liq 1 + liq 2
371.2	0.778	0.222	liq 1 + liq 2
370.2	0.767	0.233	liq 1 + liq 2
370.2	0.717	0.283	liq 1 + liq 2
370.2	0.668	0.332	liq 1 + liq 2
370.2	0.604	0.396	liq 1 + liq 2
370.4	0.585	0.415	liq 1 + liq 2
370.2	0.540	0.460	liq 1 + liq 2
370.2	0.538	0.462	liq 1 + liq 2
370.2	0.537	0.563	liq 1 + liq 2
369.2	0.326	0.674	(2) + liq 2
368.2	0.280	0.720	(2) + liq 2
368.2	0.253	0.747	(2) + liq 2
363.2	0.224	0.776	(2) + liq 2
367.2	0.212	0.788	(2) + liq 2
362.2	0.122	0.878	(2) + liq 2
359.2	0.092	0.908	(2) + liq 2
355.2	0.073	0.927	(2) + liq 2
347.7	0.036	0.964	(1) + liq 2
353.2	0.000	1.000	(1)

Compiler: A miscibility gap is observed in system.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) Furfuryl Alcohol; $C_5H_6O_2$; [98-00-0]

ORIGINAL MEASUREMENTS:

Sunier, A.A.

J. Phys. Chem. 1931, *35*, 1756-1761.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
305.6	0.8906	0.1094
319.5	0.814	0.186
326.2	0.751	0.249
331.9	0.668	0.332
337.5	0.545	0.455
340.4	0.439	0.561
341.5	0.381	0.619
344.6	0.262	0.738
345.8	0.215	0.785

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from methanol.

(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0002. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. <u>1926</u>, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
279.5	0.873	0.127
287.5	0.836	0.164
297.4	0.773	0.227
305.8	0.700	0.300
312.5	0.634	0.366
312.5	0.634	0.366
320.4	0.535	0.465
326.1	0.460	0.540
331.7	0.377	0.623
335.9	0.307	0.693
340.4	0.230	0.770
342.7	0.195	0.805

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gentle rotation to thoroughly mix contents. Bath temperature was slowly increased and solubility visually determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.

(2) Purity and source not specified, was stored over calcium chloride and sodium amalgam, distilled collecting fraction at 56.1 °C.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.717	0.283

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

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

(2) Reagent Grade or better, source not specified, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Mahieu, J.

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

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2[a]	x_1[a]
25.0	0.714	0.286

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

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Ward, H.L.

J. Phys. Chem. 1926, *30*, 1316-1333.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
276.1	0.839	0.161	333.4	0.322	0.678
287.0	0.781	0.219	338.5	0.249	0.751
297.2	0.710	0.290	345.0	0.148	0.852
318.5	0.512	0.488			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.
(2) Purity and source not specified, was fractionally distilled once before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:

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

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

ORIGINAL MEASUREMENTS:

Srivastava, R.D.; Gupta, P.D.

J. Indian Chem. Soc. 1967, *44*, 960-963.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
288.0	0.7767	0.2233	302.0	0.6723	0.3277
293.0	0.7417	0.2583	302.6	0.6645	0.3355
298.0	0.7044	0.2956	308.2	0.6224	0.3776
300.2	0.7044	0.2956			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was recrystallized and sublimed.

(2) Purity not given, British Drug Houses, was dried and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 3 % (relative error, Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	Kremann, R. *Monatsch. Chem.* 1904, *25*, 1271-1292.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
276.2	1.000	0.000	(2)
274.2	0.957	0.043	(2)
271.2	0.911	0.089	(2)
269.7	0.850	0.150	(1)
285.2	0.786	0.214	(1)
292.5	0.736	0.264	(1)
303.2	0.653	0.347	(1)
307.2	0.628	0.372	(1)
313.2	0.571	0.429	(1)
318.2	0.521	0.479	(1)
322.2	0.478	0.522	(1)
323.2	0.458	0.542	(1)
327.2	0.417	0.583	(1)
329.2	0.386	0.614	(1)
337.2	0.275	0.725	(1)
343.2	0.192	0.808	(1)
354.2	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.137 and T/K = 267.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Aniline; C_6H_7N; [62-53-3]	Ward, H.L. *J. Phys. Chem.* 1926, *30*, 1316-1333.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
273.8	0.930	0.070	310.6	0.723	0.277
283.8	0.899	0.101	324.0	0.551	0.449
286.1	0.891	0.109	334.0	0.374	0.626
295.2	0.846	0.154	338.6	0.287	0.713
303.1	0.792	0.208	347.6	0.119	0.881

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not specified, was recrystallized several times from methanol to give a melting temperature of 80.05-80.10 °C.
(2) Technical Grade, source not given, was distilled twice. Product showed slight color.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: to 3 significant figs. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Thiophene; C_4H_4S; [110-02-1]	Choi, P.B.; McLaughlin, E. *Ind. Eng. Chem. Fundam.* 1983, *22*, 46-51.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
303.2	0.6412	0.3588	336.8	0.2628	0.7372
318.2	0.4989	0.5011	341.1	0.1947	0.8053
322.7	0.4490	0.5510	348.1	0.0833	0.9167

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Pyridine; C_5H_5N; [110-86-1]	Choi, P.B.; McLaughlin, E. *Ind. Eng. Chem. Fundam.* 1983, *22*, 46-51.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
297.6	0.6968	0.3032	337.2	0.2578	0.7422
325.3	0.4252	0.5748	344.4	0.1430	0.8570
333.2	0.3192	0.6808			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Eastman Kodiak Chemical Company, Rochester, New York, USA, was passed over activated alumina and then recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2-Nitrobenzaldehyde; $C_7H_5NO_3$; [552-89-6]	Shinomiya, C. *Nihon Kagakkai Shi.* 1939, *60*, 170-182.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
311.2	1.000	0.000	326.2	0.446	0.554
308.2	0.801	0.199	331.7	0.379	0.621
303.2	0.701	0.299	344.2	0.181	0.819
315.2	0.582	0.418	353.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 3-Nitrobenzaldehyde; $C_7H_5NO_3$; [99-61-6]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

Nihon Kagakkai Shi. 1939, *60*, 170-182.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
330.2	1.000	0.000	(2)
325.7	0.903	0.097	(2)
319.7	0.784	0.216	(2)
315.7	0.656	0.344	(2)
312.7	0.624	0.376	(2)
310.7	0.603	0.397	(2)
310.2	0.599	0.401	Eutectic
316.7	0.525	0.475	(1)
321.7	0.469	0.531	(1)
322.7	0.451	0.549	(1)
330.7	0.358	0.642	(1)
332.2	0.356	0.644	(1)
345.2	0.173	0.837	(1)
353.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 4-Nitrobenzaldehyde; $C_7H_5NO_3$; [555-16-8]	Shinomiya, C. *Nihon Kagakkai Shi.* 1939, *60*, 170-182.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
378.2	1.000	0.000	(2)
372.7	0.851	0.149	(2)
367.2	0.727	0.273	(2)
358.7	0.587	0.413	(2)
356.2	0.542	0.458	(2)
350.7	0.446	0.554	(2)
339.2	0.395	0.605	(2)
331.2	0.355	0.645	(1)
336.2	0.333	0.667	(1)
333.7	0.330	0.670	(1)
336.7	0.278	0.722	(1)
339.2	0.257	0.743	(1)
342.2	0.208	0.792	(1)
342.2	0.185	0.815	(1)
348.7	0.090	0.910	(1)
352.2	0.030	0.970	(1)
353.7	0.010	0.990	(1)
353.2	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.64 and T/K = 331.6.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Chloro-3-nitrobenzene; $C_7H_5NO_3$; [121-73-3]	Shinomiya, C. *Nihon Kagakkai Shi.* 1939, *60*, 170-182.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
318.2	1.000	0.000	(2)
315.2	0.926	0.074	(2)
312.2	0.824	0.176	(2)
308.2	0.754	0.246	(2)
305.2	0.715	0.285	(2)
312.2	0.536	0.464	(1)
318.7	0.464	0.536	(1)
339.7	0.217	0.783	(1)
347.2	0.110	0.890	(1)
353.2	0.000	1.000	(1)

Phase diagram depicted in paper shows a simple eutectic system.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 1-Chloro-4-nitrobenzene; $C_7H_5NO_3$; [100-00-5]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

Nihon Kagakkai Shi. <u>1939</u>, *60*, 170-182.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
356.7	1.000	0.000	(2)
347.2	0.827	0.173	(2)
332.2	0.669	0.331	(2)
334.2	0.659	0.341	(2)
329.2	0.637	0.363	(2)
326.2	0.601	0.399	(2)
322.2	0.573	0.427	(2)
317.2	0.532	0.468	(2)
319.2	0.431	0.569	(1)
322.7	0.424	0.576	(1)
326.2	0.375	0.625	(1)
329.2	0.352	0.648	(1)
330.2	0.346	0.654	(1)
331.2	0.328	0.672	(1)
342.2	0.230	0.770	(1)
346.2	0.179	0.821	(1)
353.2	0.000	1.000	(1)

Phase diagram depicted in paper shows a simple eutectic system.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.7 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 2,4-Dinitroaniline; $C_6H_5N_3O_4$; [97-02-9]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

Nihon Kagakkai Shi. 1938, *59*, 922-926.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
452.7	1.000	0.000
446.7	0.942	0.058
444.2	0.867	0.133
440.7	0.774	0.226
438.2	0.737	0.263
431.2	0.637	0.363
427.2	0.587	0.413
427.2	0.554	0.446
427.2	0.512	0.488
427.2	0.491	0.509
426.7	0.446	0.534
425.2	0.392	0.608
423.7	0.386	0.614
413.2	0.230	0.770
404.2	0.149	0.851
354.2	0.036	0.964
353.2	0.015	0.985
353.2	0.000	1.000

Compiler: A miscibility gap is observed in system for $0.410 < x_1 < 0.510$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3]	Shinomiya, C. *Nihon Kagakkai Shi.* 1938, *59*, 922-926.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
478.2	1.000	0.000	(2)
474.7	0.908	0.092	(2)
463.7	0.720	0.280	(2)
460.7	0.691	0.309	(2)
455.2	0.604	0.396	1:1 Compound
455.2	0.520	0.480	1:1 Compound
455.2	0.507	0.493	1:1 Compound
453.2	0.377	0.623	1:1 Compound
452.7	0.301	0.699	1:1 Compound
452.2	0.287	0.713	1:1 Compound
448.2	0.240	0.760	1:1 Compound
436.7	0.121	0.879	1:1 Compound
423.2	0.086	0.914	1:1 Compound
397.2	0.038	0.962	1:1 Compound
353.2	0.000	1.000	(1)

Phase diagram depicted in paper shows formation of a 1:1 naphthalene - 3,5-dinitrobenzoic acid molecular compound having a melting point of T/K = 455.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by visually observing the temperature corresponding to the first crystal formation (or complete liquefication).	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.3 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 1,3,5-Trimethyl-2,4,6-trinitrobenzene; $C_9H_9N_3O_6$; [602-96-0]

ORIGINAL MEASUREMENTS:

Hammick, D.L.; Hellicar, A.

J. Chem. Soc. 1938, 761-763.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
505.2	1.00	0.00	(2)
502.2	0.90	0.10	(2)
493.9	0.80	0.20	(2)
489.7	0.73	0.27	(2)
478.4	0.63	0.37	(2)
465.7	0.51	0.49	(2)
450.2	0.40	0.60	(2)
433.2	0.29	0.71	(2)
408.7	0.20	0.80	(2)
395.2	0.16	0.84	(2)
368.5	0.10	0.90	(2)
351.7	0.02	0.98	(1)
353.2	0.00	1.00	(1)

Phase diagram depicted in paper shows a simple eutectic system.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Temperatures of solid-liquid equilibrium were determined by the synthetic method. Weighed amounts of the two components were sealed in tubes, temperature slowly varied until a mean temperature was found at which a small crystal of the solid phase remained unchanged.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.005 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 4-Nitro-1-methylbenzene; $C_7H_7NO_2$; [99-99-0]	Kofler, A. *Z. Physik. Chem., Pt. A.* 1940, *187*, 201-210.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
325.2	1.00	0.00	(2)
320.2	0.89	0.11	(2)
314.2	0.79	0.21	(2)
307.2	0.69	0.31	(2)
303.7	0.63	0.37	(1)
306.7	0.58	0.42	(1)
318.7	0.48	0.52	(1)
328.2	0.38	0.62	(1)
335.2	0.29	0.71	(1)
343.2	0.19	0.81	(1)
349.2	0.09	0.91	(1)
353.7	0.00	1.00	(1)

Compiler: Eutectic point occurs at about x_1 = 0.386 and T/K = 302.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and a hot-stage microscope. Binary mixtures prepared by weight. Melting point temperatures determined by thermal analysis method developed by the author, using a hot-stage microscope.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.01 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 4-Nitro-1-methylbenzene; $C_7H_7NO_2$; [99-99-0]	Kremann, R. *Monatsch. Chem.* 1904, *25*, 1271-1292.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
325.2	1.000	0.000	(2)
319.2	0.886	0.114	(2)
312.2	0.772	0.228	(2)
305.2	0.674	0.326	(2)
302.2	0.606	0.394	(1)
305.7	0.586	0.414	(1)
309.2	0.559	0.441	(1)
315.2	0.503	0.497	(1)
320.2	0.435	0.565	(1)
328.2	0.371	0.629	(1)
334.2	0.295	0.705	(1)
341.7	0.207	0.793	(1)
348.2	0.110	0.890	(1)
353.7	0.000	1.000	(1)

Compiler: Eutectic point occurs at about $x_1 = 0.376$ and $T/K = 301.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0]

ORIGINAL MEASUREMENTS:

Sekiguchi, K.; Suzuki, E.; Tsuda, Y.; Shirotani, K.-I.; Okamoto, K.

Chem. Pharm. Bull. 1984, *32*, 658-664.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
363.8	1.000	0.000	(2)
356.4	0.877	0.123	(2)
348.3	0.757	0.243	(2)
341.8	0.690	0.310	(2)
337.7	0.646	0.354	(2)
332.2	0.585	0.415	(2)
326.1	0.531	0.469	(2)
324.6	0.518	0.482	1:1 Compound
325.0	0.497	0.503	1:1 Compound
324.6	0.457	0.543	1:1 Compound
324.3	0.435	0.565	1:1 Compound
323.6	0.411	0.589	1:1 Compound
325.0	0.381	0.619	(1)
328.9	0.351	0.649	(1)
330.7	0.328	0.662	(1)
332.7	0.301	0.699	(1)
338.7	0.245	0.755	(1)
345.2	0.161	0.839	(1)
349.6	0.077	0.923	(1)
353.7	0.000	1.000	(1)

Compiler: Phase diagram shows formation of a 1:1 naphthalene - 1,3-dinitrobenzene molecular compound. Two eutectic points occur at about x_1 = 0.476 and T/K = 324.2 and at x_1 = 0.600 and T/K = 323.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance, differential thermal analyzer and differential scanning calorimeter.

Binary mixtures prepared by weight. Phase diagram determined by combined differential thermal analysis and differential scanning calorimetric methods, supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

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

(2) Purity and chemical source were not specified in paper, recrystallized from both ethanol and methanol before use.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1904, *25*, 1271-1292.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
360.7	1.000	0.000
356.2	0.939	0.061
352.2	0.875	0.125
348.2	0.789	0.211
339.7	0.720	0.280
333.2	0.661	0.339
326.2	0.599	0.401
323.7	0.577	0.423
323.8	0.555	0.445
323.6	0.544	0.456
323.6	0.517	0.483
324.0	0.500	0.500
324.0	0.491	0.509
323.8	0.463	0.537
323.6	0.454	0.546
323.7	0.433	0.567
324.0	0.433	0.567
325.0	0.392	0.608
325.2	0.383	0.617
324.9	0.381	0.619
328.7	0.353	0.647
329.5	0.340	0.660
334.5	0.276	0.724
337.4	0.243	0.757
340.7	0.205	0.795
345.7	0.121	0.879
348.2	0.089	0.911
351.7	0.032	0.968
353.8	0.000	1.000

Phase diagram suggests formation of a 1:1 naphthalene - 1,3-dinitrobenzene molecular compound having a melting temperature of circa T/K = 324.0. Two eutectic points occur at about x_1 = 0.42 and T/K = 323.6 and at x_1 = 0.60 and T/K = 323.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 1,3,5-Trinitrobenzene; $C_6H_3N_3O_6$; [99-35-4]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1904, *25*, 1271-1292.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
395.2	1.000	0.000	(2)
393.2	0.971	0.029	(2)
389.2	0.915	0.085	(2)
401.2	0.825	0.175	1:1 Compound
413.7	0.731	0.269	1:1 Compound
419.7	0.649	0.351	1:1 Compound
424.2	0.540	0.460	1:1 Compound
424.2	0.459	0.541	1:1 Compound
424.0	0.436	0.564	1:1 Compound
423.7	0.417	0.583	1:1 Compound
422.2	0.390	0.610	1:1 Compound
421.7	0.375	0.625	1:1 Compound
420.7	0.356	0.644	1:1 Compound
418.2	0.318	0.682	1:1 Compound
414.2	0.287	0.713	1:1 Compound
409.7	0.246	0.754	1:1 Compound
402.2	0.197	0.803	1:1 Compound
391.2	0.148	0.852	1:1 Compound
381.2	0.127	0.873	1:1 Compound
363.2	0.077	0.923	1:1 Compound
351.2	0.051	0.949	Eutectic
352.7	0.029	0.971	(1)
354.2	0.000	1.000	(1)

Phase diagram suggests formation of a 1:1 naphthalene - 1,3,5-trinitrobenzene molecular compound having a melting point of circa T/K = 425.7. Two eutectic points occur at about x_1 = 0.11 and T/K = 387.3 and at x_1 = 0.95 and T/K = 351.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 2-Nitrophenol; $C_6H_5NO_3$; [88-75-5]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1904, *25*, 1271-1292.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
318.2	1.000	0.000	(2)
315.2	0.943	0.057	(2)
312.2	0.880	0.120	(2)
307.2	0.765	0.235	(2)
304.2	0.712	0.288	(2)
304.2	0.689	0.311	(1)
305.2	0.686	0.314	(1)
307.2	0.659	0.341	(1)
308.0	0.654	0.346	(1)
312.7	0.610	0.390	(1)
317.2	0.560	0.440	(1)
322.2	0.493	0.507	(1)
325.7	0.451	0.549	(1)
329.2	0.402	0.598	(1)
343.7	0.340	0.660	(1)
337.2	0.280	0.720	(1)
343.2	0.175	0.825	(1)
350.2	0.075	0.925	(1)
353.7	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 4-Nitrophenol; $C_6H_5NO_3$; [100-02-7]	Kremann, R. *Monatsch. Chem.* 1904, *25*, 1271-1292.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
386.2	1.000	0.000	(2)
380.2	0.900	0.100	(2)
375.2	0.799	0.201	(2)
368.2	0.686	0.314	(2)
365.2	0.607	0.393	(2)
362.2	0.554	0.446	(2)
360.2	0.496	0.504	(2)
358.2	0.461	0.539	(2)
357.5	0.446	0.554	(2)
355.5	0.408	0.592	(2)
354.2	0.381	0.619	(2)
348.2	0.269	0.731	(2)
348.2	0.181	0.819	(1)
351.2	0.063	0.937	(1)
353.7	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,4-Dinitro-1-methylbenzene; $C_7H_6N_2O_4$; [121-14-2]	Kofler, A. *Z. Physik. Chem., Pt. A.* <u>1940</u>, *187*, 201-210.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
343.7	1.00	0.00	(2)
338.2	0.86	0.14	(2)
329.7	0.74	0.26	(1)
329.7	0.68	0.32	1:1 Compound
331.7	0.62	0.38	1:1 Compound
333.2	0.51	0.49	1:1 Compound
333.2	0.41	0.59	1:1 Compound
332.2	0.32	0.68	(1)
340.2	0.23	0.77	(1)
345.2	0.15	0.85	(1)
350.7	0.07	0.93	(1)
353.7	0.00	1.00	(1)

Author reports formation of a 1:1 naphthalene - 2,4-dinitro-1-methylbenzene molecular compound. Two eutectic points occur at x_1 = 0.29 and T/K = 326.2, at x_1 = 0.66 and T/K = 330.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Analytical balance and a hot-stage microscope. Binary mixtures prepared by weight. Melting point temperatures determined by thermal analysis method developed by the author, using a hot-stage microscope.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.01 (Compiler).

COMPONENTS:

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

(2) 2,4-Dinitro-1-methylbenzene; $C_7H_6N_2O_4$; [121-14-2]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1904, *25*, 1271-1292.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
344.7	1.000	0.000	(2)
341.2	0.942	0.058	(2)
335.7	0.835	0.165	(2)
331.2	0.776	0.224	(2)
330.2	0.669	0.331	1:1 Compound
331.2	0.620	0.380	1:1 Compound
333.2	0.553	0.447	1:1 Compound
333.2	0.477	0.523	1:1 Compound
333.2	0.462	0.538	1:1 Compound
332.2	0.412	0.588	1:1 Compound
332.2	0.405	0.595	1:1 Compound
331.2	0.360	0.640	1:1 Compound
331.7	0.300	0.700	(1)
338.2	0.205	0.795	(1)
345.2	0.145	0.855	(1)
351.2	0.058	0.942	(1)
353.7	0.000	1.000	(1)

Compiler: Phase diagram shows formation of a 1:1 naphthalene - 2,4-dinitromethylbenzene molecular compound having a melting temperature of circa T/K = 333.2. Two eutectic points occur at about x_1 = 0.263 and T/K = 327 and at x_1 = 0.681 and T/K = 329.6.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) 2,4-Dinitrophenol; $C_6H_4N_2O_5$; [51-28-5]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1904, *25*, 1271-1292.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
383.2	1.000	0.000	(2)
377.2	0.888	0.112	(2)
369.2	0.771	0.229	(2)
363.2	0.676	0.324	(2)
362.7	0.613	0.387	1:1 Compound
364.8	0.558	0.442	1:1 Compound
364.7	0.554	0.446	1:1 Compound
365.2	0.531	0.469	1:1 Compound
365.2	0.509	0.491	1:1 Compound
365.2	0.497	0.503	1:1 Compound
365.2	0.458	0.542	1:1 Compound
365.2	0.447	0.553	1:1 Compound
364.7	0.423	0.577	1:1 Compound
363.7	0.371	0.629	1:1 Compound
363.7	0.368	0.632	1:1 Compound
362.2	0.328	0.672	1:1 Compound
361.7	0.318	0.682	1:1 Compound
360.2	0.288	0.712	1:1 Compound
352.7	0.210	0.790	1:1 Compound
347.2	0.166	0.834	1:1 Compound
346.7	0.120	0.880	(1)
349.7	0.069	0.931	(1)
352.2	0.030	0.970	(1)
353.7	0.000	1.000	(1)

Compiler: Phase diagram shows formation of a 1:1 molecular compound having a melting temperature of $T/K = 365.2$. Two eutectic points occur at about $x_1 = 0.366$ and $T/K = 361.1$ and at $x_1 = 0.858$ and $T/K = 345.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

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

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,4,6-Trinitrophenol; $C_6H_3N_3O_7$; [88-89-1]	Nigam, R.K.; Dhillon, M.S. *Indian J. Chem.* 1970, *8*, 821-825.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
395.2	1.0000	0.0000	(2)
387.2	0.9135	0.0865	1:1 Compound
404.0	0.8246	0.1754	1:1 Compound
409.2	0.7855	0.2145	1:1 Compound
416.8	0.7135	0.2865	1:1 Compound
423.0	0.6060	0.3940	1:1 Compound
424.2	0.5475	0.4525	1:1 Compound
424.1	0.4467	0.5533	1:1 Compound
421.2	0.3588	0.6412	1:1 Compound
407.4	0.1981	0.8019	1:1 Compound
381.2	0.0819	0.9181	1:1 Compound
353.4	0.0000	1.0000	(1)

Compiler: Phase diagram shows formation of a 1:1 naphthalene - 2,4,6-trinitrophenol molecular compound. The two eutectic points occur at about $x_1 = 0.059$ and $T/K = 382.6$ and at $x_1 > 0.95$ and $T/K = 345.6$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Phase diagram was determined using a thaw-melt method (described in detail detail in Rastogi and Nigam, *Proc. Natl. Inst. Sci. India* 1960, *26*, 184).	(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 ± 0.1. x_1: ± 0.0001 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Isoquinoline; C_9H_7N; [119-65-3]	Kravchenko, V.M.; Pastukhova, I.S. *J. Appl. Chem. U.S.S.R.* <u>1952</u>, *25*, 343-350. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
297.2	297.2	1.000	0.000
301.2	299.7	0.953	0.047
306.2	304.2	0.891	0.109
314.2	311.2	0.792	0.208
319.7	316.2	0.703	0.297
326.7	323.2	0.588	0.412
331.2	327.2	0.500	0.500
336.7	333.2	0.398	0.602
341.2	338.2	0.300	0.700
345.2	343.2	0.200	0.800
349.2	348.2	0.096	0.904
353.2	353.2	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a complete series of solid solutions. Melting points of binary mixtures lie between those of the two pure components. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
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 distilled before use.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) Perfluoro-dibutyl ether; $C_8F_{18}O$
[308-48-5]

ORIGINAL MEASUREMENTS:

Simons, J.H.; Linevsky, M.J.

J. Am. Chem. Soc. 1952, *74*, 4750-4751.

VARIABLES:

T/K = 298 and 308

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9974	0.00257
35.0	0.9960	0.00402

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations placed in special solubility flask and equilibrated in a constant temperature bath for 48 hours. The entire saturated solution was withdrawn by suction. Solubility based upon weight of undissolved solid, which remained in the solubility flask after solution was removed.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given, was recrystallized two times from ethanol.

(2) Purity and specific isomer not specified, was synthesized by authors and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

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

(2) Perfluoro-tripropylamine; $C_9F_{21}N$
[338-83-0]

ORIGINAL MEASUREMENTS:

Simons, J.H.; Linevsky, M.J.

J. Am. Chem. Soc. 1952, *74*, 4750-4751.

VARIABLES:

T/K = 298 and 308

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9970	0.00300
35.0	0.9954	0.00461

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations placed in special solubility flask and equilibrated in a constant temperature bath for 48 hours. The entire saturated solution was withdrawn by suction. Solubility based upon weight of undissolved solid, which remained in the solubility flask after solution was removed.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given, was recrystallized two times from ethanol.

(2) Purity and specific isomer not specified, was synthesized by authors and distilled shortly before use.

ESTIMATED ERRORS:

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

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

Zhur. Fiz. Khim. 1939, *13*, 133-145.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
274.2	0.890	0.061	295.2	0.525	0.283
270.8	0.858	0.097	306.9	0.470	0.363
270.6	0.854	0.064	317.2	0.384	0.472
270.0	0.844	0.075	327.2	0.299	0.589
233.2	0.829	0.092	335.2	0.217	0.708
267.9	0.822	0.100	250.4	0.609	0.047
269.4	0.802	0.122	249.6	0.598	0.061
272.4	0.780	0.145	260.2	0.582	0.089
284.2	0.721	0.210	284.2	0.503	0.210
265.2	0.788	0.044	241.9	0.527	0.026
263.6	0.769	0.066	240.7	0.516	0.047
261.7	0.753	0.087	239.7	0.514	0.050
263.2	0.735	0.109	247.2	0.507	0.063
272.7	0.705	0.143	259.0	0.494	0.087
283.4	0.654	0.206	273.6	0.464	0.144
296.2	0.590	0.281	283.4	0.429	0.207
268.2	0.708	0.033	296.3	0.390	0.279
256.6	0.688	0.060	307.6	0.337	0.377
255.7	0.673	0.083	318.0	0.289	0.466
260.2	0.661	0.098	326.9	0.225	0.584
273.8	0.624	0.144	335.4	0.158	0.708
283.7	0.582	0.207	346.2	0.078	0.856

(Continued on next page)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_2: ± 0.002 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

Zhur. Fiz. Khim. 1939, *13*, 133-145.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES (Continuation)

T/K	x_2	x_1
230.1	0.425	0.034
230.0	0.421	0.043
235.2	0.417	0.052
248.2	0.411	0.066
283.4	0.349	0.207
216.4	0.326	0.028
215.9	0.323	0.038
224.5	0.321	0.046
234.2	0.316	0.058
246.9	0.313	0.071
258.2	0.305	0.092
273.7	0.286	0.147
284.2	0.267	0.206
295.6	0.243	0.278
194.6	0.224	0.016
194.2	0.222	0.025
205.7	0.220	0.033
224.4	0.216	0.050
247.8	0.210	0.076
260.1	0.205	0.102
274.0	0.194	0.148
282.9	0.181	0.205
295.2	0.166	0.272
307.0	0.145	0.363
318.2	0.120	0.470
327.3	0.092	0.587
335.2	0.065	0.713
172.2	0.110	0.013
192.0	0.114	0.026
225.4	0.110	0.051
259.7	0.104	0.103
273.2	0.098	0.150
283.4	0.092	0.208
172.7	0.149	0.015
170.2	0.128	0.014
187.6	0.126	0.023

COMPONENTS:

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

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

(3) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.

Zhur. Fiz. Khim. 1939, *13*, 989-1000.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
327.9	0.335	0.603	317.9	0.242	0.492
318.2	0.437	0.482	308.3	0.294	0.383
307.8	0.529	0.374	293.0	0.350	0.265
293.2	0.620	0.266	269.2	0.410	0.137
268.3	0.729	0.136	253.0	0.433	0.089
265.4	0.740	0.124	239.2	0.447	0.060
262.8	0.752	0.110	237.2	0.451	0.051
263.6	0.761	0.099	238.9	0.458	0.037
266.2	0.800	0.053	327.2	0.102	0.630
338.7	0.162	0.759	317.5	0.140	0.495
328.1	0.259	0.614	308.7	0.170	0.387
318.6	0.344	0.487	293.0	0.203	0.265
308.1	0.418	0.377	269.2	0.239	0.136
293.4	0.491	0.268	254.0	0.253	0.088
267.7	0.584	0.131	238.2	0.262	0.055
254.2	0.607	0.095	219.2	0.268	0.032
251.2	0.409	0.087	213.0	0.273	0.016
251.9	0.627	0.077	292.7	0.087	0.266
253.2	0.633	0.057	276.4	0.099	0.168
255.0	0.642	0.042	269.2	0.102	0.142
339.2	0.110	0.768	253.2	0.108	0.089
328.4	0.181	0.620	237.5	0.113	0.051
220.4	0.116	0.023	220.4	0.115	0.033
212.3	0.273	0.023	220.3	0.275	0.032

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_2: ± 0.002 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

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

(3) Isoquinoline; C_9H_7N; [119-65-3]

ORIGINAL MEASUREMENTS:

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

Zhur. Fiz. Khim. 1953, *27*, 822-834.

VARIABLES:

Temperature, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
288.0	0.329	0.085	340.3	0.182	0.749
299.7	0.296	0.178	268.2	0.846	0.063
309.2	0.262	0.273	267.2	0.832	0.079
323.9	0.197	0.454	264.7	0.817	0.096
337.9	0.118	0.672	274.7	0.776	0.142
275.9	0.516	0.082	286.0	0.707	0.217
288.2	0.473	0.157	309.5	0.544	0.398
301.4	0.420	0.252	269.8	0.880	0.062
324.3	0.285	0.492	268.2	0.860	0.083
335.2	0.197	0.649	265.7	0.834	0.110
257.8	0.674	0.071	268.2	0.810	0.136
269.5	0.654	0.100	284.7	0.736	0.215
293.9	0.553	0.239	309.5	0.573	0.389
315.8	0.418	0.424	328.9	0.375	0.600
332.8	0.265	0.635			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

SOURCE AND PURITY OF MATERIALS:

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

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

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

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_2: ± 0.002 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

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

(2) Acetonitrile; C_2H_3N; [75-05-8]

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

ORIGINAL MEASUREMENTS:

Khossravi, D.; Connors, K.A.

J. Pharm. Sci. 1992, *81*, 371-379.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	c_1/(mol dm^{-3})
0.0000	2.01×10^{-4}
0.0096	2.55×10^{-4}
0.0228	3.49×10^{-4}
0.0330	4.66×10^{-4}
0.0469	6.45×10^{-4}
0.0594	10.23×10^{-4}
0.0733	14.17×10^{-4}
0.0887	22.44×10^{-4}
0.1125	50.23×10^{-4}
0.1316	71.64×10^{-4}
0.1898	27.45×10^{-3}
0.2280	51.16×10^{-3}

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with ultraviolet detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass ampules and allowed to equilibrate in a constant temperature water bath for 48 hours. Aliquots of the saturated solutions were removed, filtered through a 0.22 micrometer polytetrafluoroethylene membrane filter, transfered to a volumetric flask, and diluted quantitatively to the mark. Solute concentrations were determined using reversed-phase HPLC with uv detection at 274 nm. 4-Butylbenzoic acid served as the internal standard.

SOURCE AND PURITY OF MATERIALS:

(1) Purified Grade, Mallinckrodt, Paris, Kentucky, USA, was used as received.

(2) HPLC grade, EM Science, Gibbstown, New Jersey, USA, was used as received from the chemical supplier.

(3) Was purified with a Sybron/Barnstead PCS system consisting of prefilter, organic ion exchange, and microfilter (0.2 micrometer) cartridges.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Khossravi, D.; Connors, K.A.

J. Pharm. Sci. 1992, *81*, 371-379.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	c_1/(mol dm^{-3})
0.0000	2.01×10^{-4}
0.0135	2.14×10^{-4}
0.0294	2.68×10^{-4}
0.0294	2.61×10^{-4}
0.0432	2.94×10^{-4}
0.0432	3.14×10^{-4}
0.0579	3.54×10^{-4}
0.0900	5.02×10^{-4}
0.1236	7.45×10^{-4}
0.1936	18.47×10^{-4}
0.2732	50.31×10^{-4}
0.3591	13.43×10^{-3}
0.4588	33.22×10^{-3}

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with ultraviolet detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass ampules and allowed to equilibrate in a constant temperature water bath for 48 hours. Aliquots of the saturated solutions were removed, filtered through a 0.22 micrometer polytetrafluoroethylene membrane filter, transfered to a volumetric flask, and diluted quantitatively to the mark. Solute concentrations were determined using reversed-phase HPLC with uv detection at 274 nm. 4-Butylbenzoic acid served as the internal standard.

SOURCE AND PURITY OF MATERIALS:

(1) Purified Grade, Mallinckrodt, Paris, Kentucky, USA, was used as received.

(2) HPLC grade, J.T. Baker Chemical Company, Phillipsburg, New Jersey, USA, was used as received.

(3) Was purified with a Sybron/Barnstead PCS system consisting of prefilter, organic ion exchange, and microfilter (0.2 micrometer) cartridges.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 5 % (relative error; compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Sarker, M.; Wilson, D.

J. Tennessee Acad. Sci. 1986, *61*, 69-74.

VARIABLES:

T/K = Ambient Room Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, $c_1/(\text{mg L}^{-1})$, expressed in terms of the equation: $c_1/(\text{mg L}^{-1}) = 36.5\ (1 + 3.8 \times 10^5\ x_2^{3.86})$

Mole fraction compositions of 1-propanol ranged between $x_2 = 0.001$ to $x_2 = 0.10$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Gas chromatographic equipped with flame ionization detection.

Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Concentrations determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given.

(3) Purity and chemical source not given.

ESTIMATED ERRORS:

T/K: Unknown.
x_2: ± 0.001 (Compiler).
x_1: ± 8 % (Relative error; Compiler).

COMPONENTS:

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

(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

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

ORIGINAL MEASUREMENTS:

Sarker, M.; Wilson, D.

J. Tennessee Acad. Sci. 1986, *61*, 69-74.

VARIABLES:

T/K = Ambient Room Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, $c_1/(\text{mg L}^{-1})$, expressed in terms of the equation: $c_1/(\text{mg L}^{-1}) = 36.5\ (1 + 2.0 \times 10^{10}\ x_2^{3.16})$

Mole fraction compositions of 1-hexanol ranged between $x_2 = 0.0001$ to $x_2 = 0.0004$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Gas chromatographic equipped with flame ionization detection.

Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Concentrations determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given.

(3) Purity and chemical source not given.

ESTIMATED ERRORS:

T/K: Unknown.
x_2: ± 0.0001 (Compiler).
x_1: ± 8 % (Relative error; Compiler).

COMPONENTS:

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

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

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

ORIGINAL MEASUREMENTS:

Sarker, M.; Wilson, D.

J. Tennessee Acad. Sci. 1986, *61*, 69-74.

VARIABLES:

T/K = Ambient Room Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, c_1/(mg L^{-1}), expressed in terms of the equation: $c_1/(\text{mg L}^{-1}) = 36.5\ (1 + 6.7 \times 10^3\ x_2^{2.53})$

Mole fraction compositions of 2-propanone ranged between $x_2 = 0.01$ to $x_2 = 0.10$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Gas chromatographic equipped with flame ionization detection.

Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Concentrations determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given.

(3) Purity and chemical source not given.

ESTIMATED ERRORS:

T/K: Unknown.
x_2: ± 0.01 (Compiler).
x_1: ± 8 % (Relative error; Compiler).

COMPONENTS:

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

(2) 2-Butanone; C_4H_8O; [78-93-3]

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

ORIGINAL MEASUREMENTS:

Sarker, M.; Wilson, D.

J. Tennessee Acad. Sci. 1986, *61*, 69-74.

VARIABLES:

T/K = Ambient Room Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, c_1/(mg L^{-1}), expressed in terms of the equation: $c_1/(\text{mg L}^{-1}) = 36.5\ (1 + 3.4 \times 10^4\ x_2^{2.45})$

Mole fraction compositions of 2-butanone ranged between $x_2 = 0.01$ to $x_2 = 0.02$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Gas chromatographic equipped with flame ionization detection.

Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Concentrations determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given.

(3) Purity and chemical source not given.

ESTIMATED ERRORS:

T/K: Unknown.
x_2: ± 0.01 (Compiler).
x_1: ± 8 % (Relative error; Compiler).

COMPONENTS:

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

(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Khossravi, D.; Connors, K.A.

J. Pharm. Sci. 1992, *81*, 371-379.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_2^{(s)}$	c_1/(mol dm^{-3})	$x_2^{(s)}$	c_1/(mol dm^{-3})
0.0000	2.01×10^{-4}	0.4300	94.95×10^{-4}
0.0084	2.16×10^{-4}	0.5640	20.19×10^{-3}
0.0167	2.38×10^{-4}	0.5867	23.98×10^{-3}
0.0257	2.61×10^{-4}	1.0000	85.04×10^{-3}
0.0347	2.91×10^{-4}		
0.0444	3.24×10^{-4}		
0.0540	3.50×10^{-4}		
0.0748	4.28×10^{-4}		
0.0973	5.38×10^{-4}		
0.1217	7.12×10^{-4}		
0.1483	9.25×10^{-4}		
0.1773	12.47×10^{-4}		
0.2443	23.67×10^{-4}		
0.3266	47.53×10^{-4}		

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with ultraviolet detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass ampules and allowed to equilibrate in a constant temperature water bath for 48 hours. Aliquots of the saturated solutions were removed, filtered through a 0.22 micrometer polytetrafluoroethylene membrane filter, transfered to a volumetric flask, and diluted quantitatively to the mark. Solute concentrations were determined using reversed-phase HPLC with uv detection at 274 nm. 4-Butylbenzoic acid served as the internal standard.

SOURCE AND PURITY OF MATERIALS:

(1) Purified Grade, Mallinckrodt, Paris, Kentucky, USA, was used as received.

(2) Reagent grade, J.T. Baker Chemical, Company, Phillipsburg, New Jersey, USA, was used as received.

(3) Was purified with a Sybron/Barnstead PCS system consisting of prefilter, organic ion exchange, and microfilter (0.2 micrometer) cartridges.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_2^{(s)}$: ± 0.0001 (compiler).
c_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sarker, M.; Wilson, D.

J. Tennessee Acad. Sci. 1986, *61*, 69-74.

VARIABLES:

T/K = Ambient Room Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, $c_1/(\text{mg L}^{-1})$, expressed in terms of the equation: $c_1/(\text{mg L}^{-1}) = 36.5\ (1 + 8.8\ x_2^{0.37})$

Mole fractions of ethyl ethanoate ranged between $x_2 = 0.001$ to $x_2 = 0.010$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Gas chromatographic equipped with flame ionization detection.

Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Concentrations determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given.

(3) Purity and chemical source not given.

ESTIMATED ERRORS:

T/K: Unknown.
x_2: ± 0.001 (Compiler).
x_1: ± 8 % (Relative error; Compiler).

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

(2) Pyridine; C_5H_5N; [110-86-1]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sarker, M.; Wilson, D.

J. Tennessee Acad. Sci. 1986, *61*, 69-74.

VARIABLES:

T/K = Ambient Room Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, $c_1/(\text{mg L}^{-1})$, expressed in terms of the equation: $c_1/(\text{mg L}^{-1}) = 36.5\ (1 + 3.5 \times 10^4\ x_2^{2.60})$

Mole fraction compositions of pyridine ranged between $x_2 = 0.01$ to $x_2 = 0.10$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Gas chromatographic equipped with flame ionization detection.

Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Concentrations determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given.

(3) Purity and chemical source not given.

ESTIMATED ERRORS:

T/K: Unknown.
x_2: ± 0.01 (Compiler).
x_1: ± 8 % (Relative error; Compiler).

PERYLENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

benzene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:

(1) Perylene; $C_{20}H_{12}$; [198-55-0]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.00037

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured fluorescence emission intensity.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Perylene; $C_{20}H_{12}$; [198-55-0]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Mishra, D.S.; Yalkowsky, S.H.

Ind. Eng. Chem. Res., 1990, *29*, 2278-2283.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
23.0	0.9604	0.0396

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent placed in screw-capped test tube and allowed to equilibrate for 3 days with gentle agitation in a constant temperature bath. Samples centrifuged for 30 minutes and concentrations were determined spectrophotometrically. Attainment of equilibrium verified by repetitive measurements 4 days later.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent grade, source not specified, was used as received.

(2) Reagent grade, source not specified, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Perylene; $C_{20}H_{12}$; [198-55-0]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.003044

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).

c_1: ± 3 % (relative error; compiler).

PHENANTHRENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
n-octadecane
cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,2,3,4-tetrahydronaphthalene
biphenyl
fluoranthene
acenaphthene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

tetrachloromethane
1,4-dibromobenzene
1-hydroperfluoroheptane
1,8-dihydroperfluorooctane
octafluoronaphthalene

G. Alcohols

ethanol
1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene
perfluoro-tri-n-butylamine
nitrobenzene
carbon disulfide
1,2-dinitrobenzene
1,3-dinitrobenzene
1,4-dinitrobenzene
1,3,5-trinitrobenzene
1,2,3,5-tetranitrobenzene
2,4-dinitromethylbenzene
2,6-dinitromethylbenzene
3,4-dinitromethylbenzene
2,4,6-trinitromethylbenzene

2,4-dinitrophenol
1-chloro-4-nitrobenzene
dibenzothiophene
thianthrene
benzoic acid
trans-cinnamic acid
2-hydroxybenzoic acid
3-hydroxybenzoic acid
6-methyl-2,3,4-trinitrophenol

J. Binary Solvent Mixtures

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Doane, E.P.; Drickamer, H.G.

J. Phys. Chem. <u>1955</u>, *59*, 454-457.

VARIABLES:

T/K = 298, Pressure

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

P/atm	x_2	x_1	*P*/atm	x_2	x_1
1	0.9674	0.0326	4300	0.9896	0.0104
500	0.9728	0.0272	7150	0.9950	0.0050
1000	0.9774	0.0226	8750	0.9964	0.0036
2000	0.9820	0.0180			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, analytical balance and high pressure equipment.

Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount of saturated solution removed, solvent evaporated to dryness, and contration determined from weight of solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purest grade, Eastman Kodak Chemical Company, Rochester, New York, USA, was used as received.

(2) Pure grade, Phillips Petroleum, was dried over phosphorous pentoxide and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 1-3 % at atmospheric pressure, and ± 10 % at the higher pressures.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. <u>1981</u>, *26*, 19-34.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.0270

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifugation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming that the dilute solution behavior extrapolates up to saturation point.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Doane, E.P.; Drickamer, H.G.

J. Phys. Chem. 1955, *59*, 454-457.

VARIABLES:

$T/K = 298$, Pressure

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

P/atm	x_2	x_1	P/atm	x_2	x_1
1	0.9599	0.0401	2000	0.9816	0.0184
500	0.9679	0.0321	3430	0.9889	0.0111
900	0.9708	0.0292	5000	0.9916	0.0084
1000	0.9728	0.0272	7000	0.9948	0.0052

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, analytical balance and high pressure equipment.

Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount of saturated solution removed, solvent evaporated to dryness, and contration determined from weight of solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purest grade, Eastman Kodak Chemical Company, Rochester, New York, USA, was used as received.

(2) Pure grade, Phillips Petroleum, was dried over phosphorous pentoxide and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 1-3 % at atmospheric pressure, and ± 10 % at the higher pressures.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) n-Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

Doane, E.P.; Drickamer, H.G.

J. Phys. Chem. 1955, *59*, 454-457.

VARIABLES:

$T/K = 298$, Pressure

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

P/atm	x_2	x_1	P/atm	x_2	x_1
1	0.9536	0.0464	3850	0.9880	0.0120
490	0.9619	0.0381	5200	0.9912	0.0088
1000	0.9716	0.0284			
1960	0.9803	0.0197			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, analytical balance and high pressure equipment.

Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount of saturated solution removed, solvent evaporated to dryness, and contration determined from weight of solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purest grade, Eastman Kodak Chemical Company, Rochester, New York, USA, was used as received.

(2) Pure grade, Phillips Petroleum, was dried over phosphorous pentoxide and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 1-3 % at atmospheric pressure, and ± 10 % at the higher pressures.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) n-Octadecane; $C_{18}H_{38}$; [593-45-3]

ORIGINAL MEASUREMENTS:

Djordjevic, N.M.

Thermochim. Acta 1991, *177*, 109-118.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
358.8	0.3685	0.6315	364.2	0.1776	0.8224
359.9	0.3333	0.6667	367.0	0.1151	0.8849
363.5	0.1919	0.8081	367.5	0.1044	0.8956
364.1	0.1814	0.8186			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter.

Mixtures (1.5 - 2.0 mg) of known concentration were weighed into aluminum pans, which were then crimped to preclude sample loss during the heating process. Solubilities determined by measuring melting points of binary mixtures using a Perkin-Elmer DSC-2 differential scanning calorimeter and scan rate of 5 K/min.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (compiler).
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.

J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.65	0.9394	0.0606	325.85	0.8470	0.1530
313.85	0.9181	0.0819	333.25	0.7570	0.2430
319.65	0.8907	0.1093	339.55	0.6432	0.3568
321.85	0.8772	0.1228			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	**EVALUATOR:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Cyclohexane; C_6H_{12}; [110-82-7]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) August, 1994

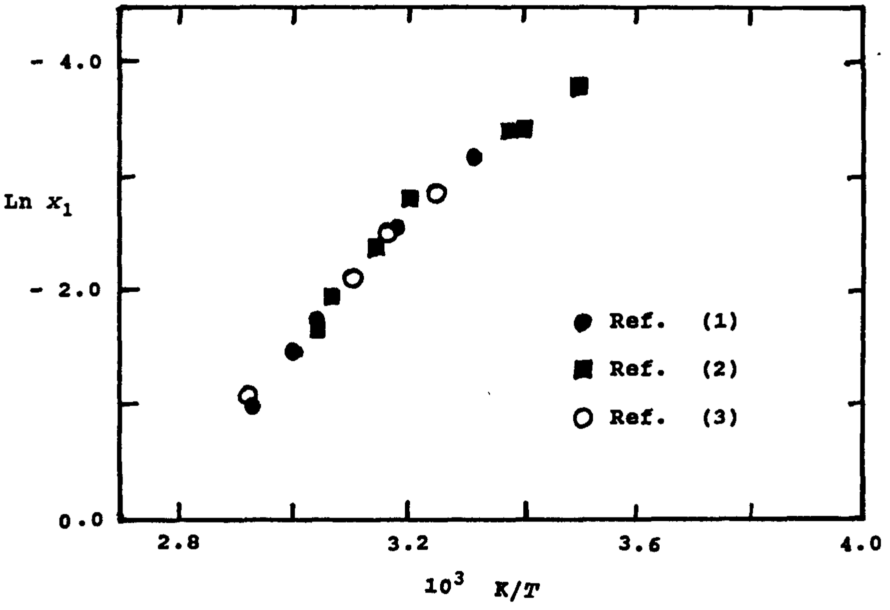
CRITICAL EVALUATION:

Phenanthrene solubilities in cyclohexane were retrieved from papers by McLaughlin and Zainal (1), Gordon and Scott (2) and Choi (3). All three studies report values at several temperatures. There is no a prior reason to exclude any of the three studies from the critical evaluation.

Regressional analysis of the experimental data as Ln x_1 versus $1/T$ yielded the following mathematical relationship:

$$\text{Ln } x_1 = -5215.6\ (1/T) + 14.1709 \qquad (r = 0.9897)$$

for variation of naphthalene solubility with absolute temperature (see graph below). Phenanthrene does exhibit a solid-solid lambda point phase transition from around 331 to 361 K (4). A graphical plot of ln x_1 versus $1/T$ is linear if the enthalpy of the transition is relatively small compared to the solute's enthalpy of fusion, as is the case here. The slight nonlinear behavior is undoubtedly attributed to the additional phase transition.



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 3854-3857.

2. Gordon, L.J.; Scott, R.L. *J. Am. Chem. Soc.* 1952, *74*, 4138-4140.

3. Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. *J. Chem. Eng. Data* 1985, *30*, 403-409.

4. Choi, P.B.; McLaughlin, E. *AIChE J.* 1983, *29*, 150-153.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 3854-3857.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.6	0.9598	0.0402	340.6	0.6253	0.3747
313.2	0.9215	0.0785			
328.8	0.8247	0.1753			
333.7	0.7606	0.2394			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.

(2) Purity, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Gordon, L.J.; Scott, R.L.

J. Am. Chem. Soc. 1952, *74*, 4138-4140.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
286.0	0.9783	0.0217	317.6	0.9061	0.0939
293.7	0.9672	0.0328	326.7	0.856	0.144
296.1	0.9663	0.0337	328.2	0.827	0.173
302.8	0.9582	0.0418	341.9	0.596	0.404
311.7	0.9392	0.0608			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Temperature of bath slowly increased at a rate not exceeding 0.5 K per minute. Solubility determined visually by noting the temperature at which the trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, was used as received.

(2) White Label, Eastman Kodak Chemical Company was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.2.
x_1: 3 significant figures (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E. *Fluid Phase Equilibr.* 1989, *44*, 305-345.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
314.4	0.8407	0.1593	337.4	0.5970	0.4030
320.1	0.7980	0.2020	341.2	0.5249	0.4751
326.2	0.7446	0.2554	345.6	0.4388	0.5612
331.9	0.6717	0.3283			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.
(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Benzene; C_6H_6; [71-43-2]	Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. *J. Chem. Eng. Data* 1985, *30*, 403-409.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
312.75	0.7185	0.2815	341.85	0.4229	0.5771
316.75	0.6872	0.3128	342.15	0.4208	0.5792
325.25	0.6042	0.3958			
334.75	0.5051	0.4949			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.2	0.7761	0.2239	331.2	0.5428	0.4572
313.4	0.7164	0.2836			
315.0	0.7010	0.2990			
323.4	0.6250	0.3750			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Bureau of Mines, USA, was passed over an alumina column with benzene as eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Speyers, C.L.

Am. J. Sci. 1902, *14*, 293-302.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.8812	0.1188	328.1	0.4675	0.5325
287.1	0.8260	0.1740	351.5	0.1802	0.8198
304.0	0.7310	0.2690			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from toluene to a melting point temperature of 100.4 °C.

(2) Purity not given, Kahlbaum, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 8 % (relative error, compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Methylbenzene; C_7H_8; [108-88-3]	Choi, P.B.; McLaughlin, E. *AIChE J.* 1983, *29*, 150-153.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
299.8	0.7541	0.2459
307.7	0.6989	0.3011
314.3	0.6487	0.3513
316.6	0.6310	0.3690
323.4	0.5717	0.4283
342.8	0.3830	0.6170
349.6	0.3039	0.6961
355.6	0.2349	0.7651
361.0	0.1651	0.8349
366.5	0.0889	0.9111

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and constant temperature bath.

Mixtures of known composition were sealed in glass ampoules, and placed in a constant temperature bath. Ampoules were slowly rotated at about 0.25 rps, while the bath temperature was increased by 0.1 K every 1,200 seconds. Temperature at which the last trace of solid disappeared was visually determined.

SOURCE AND PURITY OF MATERIALS:

(1) 98.67 % minimum, Eastern Chemical Company, USA, was purified by column chromatography and recrystallized from from toluene before use.

(2) Gold Label, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 0.0001 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.7	0.7157	0.2843	340.6	0.4319	0.5681
316.2	0.6657	0.3343			
325.8	0.5825	0.4175			
333.1	0.5113	0.4887			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.1.

x_1: $\pm$ 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Biphenyl; $C_{12}H_{10}$; [92-52-4]

ORIGINAL MEASUREMENTS:

Rai, U.S.; Shekhar, H.

Thermochim. Acta 1991, *175*, 215-227.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the orginal paper, shows that the system is a simple eutectic system. The eutectic point occurs at circa $x_1 = 0.23$ and $T/K = 333.7$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Thomas Backer & Co., Bombay, India, was purified by fractional recrystallization from ethanol.

(2) Purity not given, SOJUZ Chemicals, Moscow, USSR, was purified by recrystallization from ethanol.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.3 (Compiler).

x_1: $\pm$ 0.01 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Fluoranthene; $C_{16}H_{10}$; [206-44-0]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
383.2	1.000	0.000	(2)
375.7	0.896	0.104	(2)
365.0	0.738	0.262	(2)
358.5	0.644	0.356	(2)
353.4	0.563	0.437	(2)
347.5	0.480	0.520	(2)
346.2	0.460	0.540	Eutectic
349.6	0.391	0.609	(1)
355.3	0.294	0.706	(1)
363.8	0.156	0.844	(1)
368.7	0.065	0.935	(1)
372.5	0.000	1.000	(1)

Authors report eutectic point occurs at $x_2 = 0.460$ and at $T/K = 346.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
368.3	1.000	0.000	(2)
362.0	0.901	0.099	(2)
355.0	0.796	0.204	(2)
346.7	0.686	0.314	(2)
339.1	0.599	0.401	(2)
334.5	0.541	0.459	(2)
329.0	0.492	0.508	Eutectic
338.7	0.386	0.614	(1)
347.7	0.293	0.707	(1)
357.4	0.199	0.801	(1)
372.5	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Tetrachloromethane; CCl_4; [56-23-5]	McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 2485-2488.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.6	0.8232	0.1768	319.2	0.7080	0.2920
310.0	0.7916	0.2084			
314.0	0.7579	0.2421			
317.0	0.7336	0.2664			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.

(2) AnalaR grade, source not givne, was stored over anhydrous calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6]	Rai, U.S.; Shekhar, H. *Thermochim. Acta* 1991, *175*, 215-227.
VARIABLES:	**PREPARED BY:**
	W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the orginal paper, shows that the system is a simple eutectic system. The eutectic point occurs at circa x_1 = 0.43 and T/K = 328.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Thomas Backer & Co., Bombay, India, was purified by fractional recrystallization from ethanol.

(2) Purity not given, Fluka AG, Switzerland, was purified by crystallization from boiling ethanol.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.01 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoroheptane; C_7HF_{15}; [375-83-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Scott, R.L.

J. Phys. Chem. 1956, *60*, 674-676.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/K	x_2	x_1
25.0	0.9984	0.00160

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, a precision thermometer and uv/visible spectrometer.

Mixtures of known concentrations sealed in glass ampoules and allowed to equilibrate at a constant temperature for an unspecified length of time. Solubilities calculated from spectral absorbance data at 270 nm.

SOURCE AND PURITY OF MATERIALS:

(1) White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, was recrystallized ten times from ethanol.

(2) Purity not specified, synthesized by authors, was fractionally distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluorooctane; $C_8H_2F_{16}$; [307-99-3]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Scott, R.L.

J. Phys. Chem. 1956, *60*, 674-676.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/K	x_2	x_1
25.0	0.9951	0.00488

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, a precision thermometer and uv/visible spectrometer.

Mixtures of known concentrations sealed in glass ampoules and allowed to equilibrate at a constant temperature for an unspecified length of time. Solubilities calculated from spectral absorbance data at 270 nm.

SOURCE AND PURITY OF MATERIALS:

(1) White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, was recrystallized ten times from ethanol.

(2) Purity not specified, synthesized by authors, was fractionally distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.01.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Octafluoronaphthalene; $C_{10}F_8$; [313-72-4]	Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M. *Bull. Chem. Soc. Japan* 1985, *58*, 3643-3644.
VARIABLES:	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the original paper, shows formation of a 1:1 phenanthrene - octafluoronaphthalene molecular compound having a melting point of circa 453.2 K. Two eutectic points occur at about $x_2 = 0.09$ and $T/K = 371.2$, and at about $x_2 = 0.91$ and $T/K = 357.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Differential scanning calorimeter and an analytical balance. Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.	(1) Purity not given, Tokyo Chemical Company, Japan, was zone-refined before use. (2) Reagent grade, Tokyo Chemical Company, Japan, was recrystallized from methanol before use.
	ESTIMATED ERRORS: T/K: precision ± 0.3 (Compiler). x_1: ± 0.02 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Ethanol; C_2H_6O; [64-17-5]	Speyers, C.L. *Am. J. Sci.* 1902, *14*, 293-302.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9918	0.0082	320.2	0.9781	0.0219
284.1	0.9914	0.0086	343.4	0.9248	0.0752
305.3	0.9844	0.0156			

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 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 toluene to a melting point temperature of 100.4 °C. (2) Marked absolute, from Eimer and Amend and Chas. Cooper and Co., dried over calcium oxide and distilled before use.
	ESTIMATED ERRORS: T/K: precision ± 0.1. x_1: ± 8 % (relative error, compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$c_1/(\mathrm{mol\ dm^{-3}})$
25.0	0.4012

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
299.8	0.7541	0.2459	342.8	0.3830	0.6170
307.7	0.6989	0.3011	349.6	0.3039	0.6961
314.3	0.6487	0.3513	355.6	0.2349	0.7651
316.6	0.6310	0.3690	361.0	0.1651	0.8349
323.4	0.5717	0.4283	366.5	0.0889	0.9111

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.
(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
299.4	0.7621	0.2379	340.9	0.4093	0.5907
304.9	0.7258	0.2742	348.3	0.3243	0.6757
310.0	0.6854	0.3146	355.0	0.2459	0.7541
321.2	0.6060	0.4016			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Perfluoro-tri-n-butylamine; $C_{12}F_{27}N$; [311-89-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Scott, R.L.

J. Am. Chem. Soc. 1954, *76*, 5276-5279.

VARIABLES:

T/K = 298, 308 and 318

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/K	x_2	x_1
25.0	0.9708	0.0292
35.0	0.9511	0.0489
45.0	0.9278	0.0722

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, a precision thermometer and uv/visible spectrometer.

Mixtures of known concentrations sealed in glass ampoules and pre-equilibrated for four days at an elevated temperature. Saturated solutions were then transferred to a special solubility flask and equilibrated for three days at desired temperature. Aliquots removed, diluted ten-fold with solvent and concentrations determined spectrophotometrically at 270 nm.

SOURCE AND PURITY OF MATERIALS:

(1) White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, was recrystallized five times from ethanol to give a melting point of 101 °C.

(2) Purity not specified, Minnesota Mining & Manaufacturing Company, USA, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.02.

x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Srivastava, R.D.; Gupta, P.D.

J. Indian Chem. Soc. 1967, *44*, 960-963.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
290.2	0.7887	0.2113	301.6	0.7199	0.2801
292.0	0.7783	0.2217	302.8	0.7108	0.2892
296.0	0.7488	0.2512	308.3	0.6796	0.3204
298.2	0.7430	0.2570			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was recrystallized and sublimed.

(2) Purity not given, British Drug Houses, was dried and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Doane, E.P.; Drickamer, H.G.

J. Phys. Chem. 1955, *59*, 454-457.

VARIABLES:

T/K = 298, Pressure

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

P/atm	x_2	x_1	P/atm	x_2	x_1
1	0.765	0.235	4000	0.955	0.045
500	0.838	0.162	6000	0.971	0.029
1000	0.875	0.125	7000	0.978	0.022
2000	0.927	0.073			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, analytical balance and high pressure equipment.

Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount amount of saturated solution removed, solvent evaporated to dryness, and contration determined from weight of solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purest grade, Eastman Kodak Chemical Company, Rochester, New York, USA, was used as received.

(2) C.P. grade, J.T. Baker, was dried over phosphorous pentoxide and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 1-3 % at atmospheric pressure, and ± 10 % at the higher pressures.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,2-Dinitrobenzene; $C_6H_4N_2O_4$; [528-29-0]	Kremann, R. *Monatsch. Chem.* 1908, *29*, 863-890.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
389.2	1.000	0.000	(2)
380.3	0.829	0.171	(2)
377.2	0.769	0.231	(2)
371.2	0.669	0.331	(2)
364.7	0.573	0.427	(2)
356.7	0.488	0.512	(2)
352.7	0.433	0.567	(2)
352.2	0.431	0.569	(2)
352.2	0.335	0.665	(1)
363.4	0.293	0.807	(1)
369.7	0.107	0.893	(1)
376.2	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.61 and T/K = 348.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0]	Kremann, R. *Monatsch. Chem.* 1908, *29*, 863-890.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
362.7	1.000	0.000
360.2	0.955	0.045
356.2	0.900	0.100
353.2	0.847	0.153
349.7	0.806	0.194
345.2	0.753	0.247
342.2	0.706	0.294
338.7	0.676	0.324
335.7	0.638	0.362
331.2	0.601	0.399
326.2	0.560	0.440
321.7	0.527	0.473
321.7	0.525	0.475
324.2	0.500	0.500
326.2	0.482	0.518
331.2	0.468	0.532
328.7	0.467	0.533
330.2	0.455	0.545
333.2	0.445	0.555
335.2	0.432	0.568
337.9	0.421	0.579
338.2	0.412	0.588
343.2	0.368	0.632
350.2	0.308	0.692
357.7	0.237	0.763

T/K	x_2	x_1
362.2	0.179	0.821
369.2	0.103	0.897
373.2	0.048	0.952
376.7	0.000	1.000

Compiler: Eutectic point occurs at about x_1 = 0.482 and T/K = 320.6.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,4-Dinitrobenzene; $C_6H_4N_2O_4$; [100-25-4]	Kremann, R. *Monatsch. Chem.* <u>1908</u>, *29*, 863-890.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
445.2	1.000	0.000	(2)
443.5	0.959	0.041	(2)
441.2	0.920	0.080	(2)
438.2	0.872	0.128	(2)
433.2	0.808	0.192	(2)
428.7	0.752	0.248	(2)
428.2	0.694	0.306	(2)
423.7	0.651	0.349	(2)
419.5	0.616	0.384	(2)
410.8	0.586	0.416	(2)
402.7	0.519	0.481	(2)
397.2	0.488	0.512	(2)
392.2	0.461	0.539	(2)
386.2	0.429	0.571	(2)
377.2	0.386	0.614	(2)
357.2	0.312	0.688	(2)
354.2	0.304	0.696	(2)
352.2	0.296	0.706	(2)
353.5	0.285	0.715	(1)
354.2	0.245	0.755	(1)
353.7	0.238	0.762	(1)
354.2	0.225	0.775	(1)
362.7	0.156	0.844	(1)
367.2	0.109	0.891	(1)
371.5	0.059	0.941	(1)
376.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,3,5-Trinitrobenzene; $C_6H_3N_3O_6$; [99-35-4]	Kremann, R. *Monatsch. Chem.* 1908, *29*, 863-890.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
394.2	1.000	0.000	(2)
384.2	0.883	0.117	(2)
379.2	0.815	0.185	(2)
388.2	0.729	0.271	1:1 Compound
397.2	0.579	0.421	1:1 Compound
398.2	0.471	0.529	1:1 Compound
397.2	0.419	0.581	1:1 Compound
393.2	0.355	0.645	1:1 Compound
390.2	0.318	0.682	1:1 Compound
384.2	0.272	0.728	1:1 Compound
375.2	0.213	0.787	1:1 Compound
364.2	0.174	0.826	1:1 Compound
364.2	0.144	0.856	(1)
367.2	0.122	0.878	(1)
370.2	0.085	0.915	(1)
373.2	0.058	0.942	(1)
376.2	0.000	1.000	(1)

Phase diagram suggests formation of a 1:1 phenanthrene - 1,3,5-trinitrobenzene molecular compound having a melting point of circa T/K = 398.2. The two eutectic points occur at x_1 = 0.21 and T/K = 377.9 and at x_1 = 0.845 and T/K = 362.9.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.5 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 1,2,3,5-Tetranitrobenzene; $C_6H_2N_4O_8$; [3698-53-1]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

J. Chem. Soc. Japan 1940, *15*, 259-270.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Phases
399.2	1.000	0.000	(2)
394.2	0.921	0.079	(2) + liq 1
394.2	0.815	0.185	liq 1 + liq 2
394.2	0.810	0.190	liq 1 + liq 2
396.5	0.720	0.280	liq 1 + liq 2
396.7	0.696	0.304	liq 1 + liq 2
398.2	0.623	0.377	liq 1 + liq 2
397.7	0.575	0.425	liq 1 + liq 2
396.7	0.549	0.451	liq 1 + liq 2
396.2	0.537	0.463	liq 1 + liq 2
395.7	0.485	0.515	liq 1 + liq 2
393.7	0.483	0.517	liq 1 + liq 2
391.2	0.413	0.587	(2) + liq
391.2	0.402	0.598	(2) + liq
384.7	0.320	0.680	1:1 Compound + liq
372.2	0.238	0.762	1:1 Compound + liq
364.2	0.207	0.793	1:1 Compound + liq
360.2	0.136	0.864	(1) + liq
363.2	0.114	0.886	(1) + liq
373.7	0.000	1.000	(1)

Author reports formation of an incongruently melting 1:1 phenanthrene - 1,2,3,5-tetranitrobenzene compound, and a 2:3 phenanthrene - 1,2,3,5-tetranitrobenzene molecular compound having a melting point temperature of 398.2 K. Two eutectic points occur at x_1 = 0.120 and T/K = 388.2, and at x_1 = 0.822 and T/K = 352.2. A pertectic point occurs at x_1 = 0.615 and T/K = 388.2.

Compiler: From a thermodynamic viewpoint, phase diagram is more in agreement with with formation of a 1:1 molecular compound, with the existence of a peritectic point at x_1 = 0.615 and T/K = 388.2 and a miscibility gap at higher temperature, with a monotectic point close to x_1 = 0.12 and T/K = 392, and an eutectic point at x_1 = 0.822 and T/K = 352.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 2,4-Dinitro-1-methylbenzene; $C_7H_6N_2O_4$; [121-14-2]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1908, *29*, 863-890.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
342.2	1.000	0.000
341.2	0.968	0.032
338.7	0.924	0.076
337.2	0.889	0.111
334.7	0.854	0.146
333.2	0.819	0.181
331.2	0.791	0.209
329.2	0.756	0.244
327.7	0.733	0.267
326.2	0.716	0.284
324.2	0.693	0.307
322.2	0.658	0.342
319.9	0.638	0.362
317.2	0.610	0.390
314.2	0.580	0.420
310.7	0.557	0.443
313.2	0.544	0.456
315.2	0.532	0.468
317.7	0.511	0.489
319.2	0.508	0.492
326.2	0.471	0.529
332.7	0.427	0.573
336.2	0.402	0.598
341.2	0.372	0.628
346.7	0.334	0.666

T/K	x_2	x_1
351.2	0.293	0.707
354.7	0.262	0.738
360.2	0.210	0.790
365.7	0.151	0.849
368.2	0.122	0.878
371.2	0.076	0.924
376.7	0.000	1.000

Compiler: Eutectic point occurs at about $x_1 = 0.447$ and $T/K = 310.6$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 2,6-Dinitro-1-methylbenzene; $C_7H_6N_2O_4$; [606-20-2]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1908, *29*, 863-890.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
338.2	1.000	0.000	(2)
337.2	0.979	0.021	(2)
333.7	0.917	0.083	(2)
330.2	0.848	0.152	(2)
327.2	0.797	0.203	(2)
326.2	0.763	0.237	(2)
321.2	0.720	0.280	(2)
318.2	0.683	0.317	(2)
313.2	0.635	0.365	(2)
317.2	0.588	0.412	(1)
321.2	0.574	0.426	(1)
322.2	0.558	0.442	(1)
326.2	0.540	0.460	(1)
325.2	0.535	0.465	(1)
330.7	0.506	0.494	(1)
336.2	0.462	0.538	(1)
341.2	0.422	0.578	(1)
345.2	0.380	0.620	(1)
348.7	0.338	0.662	(1)
354.7	0.277	0.723	(1)
360.7	0.213	0.787	(1)
365.2	0.153	0.847	(1)
370.4	0.088	0.912	(1)
373.7	0.048	0.952	(1)
376.7	0.000	1.000	(1)

Compiler: Eutectic point occurs at about $x_1 = 0.375$ and $T/\mathrm{K} = 311.7$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 3,4-Dinitro-1-methylbenzene; $C_7H_6N_2O_4$; [610-39-9]	Kremann, R. *Monatsch. Chem.* 1908, *29*, 863-890.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
332.2	1.000	0.000	(2)
324.7	0.875	0.125	(2)
322.2	0.853	0.147	(2)
320.2	0.830	0.170	(2)
317.2	0.785	0.215	(2)
313.2	0.724	0.276	(2)
309.2	0.679	0.321	(2)
307.2	0.672	0.328	(2)
316.0	0.581	0.419	(1)
324.1	0.547	0.453	(1)
328.2	0.504	0.496	(1)
330.8	0.489	0.511	(1)
334.2	0.457	0.543	(1)
342.2	0.406	0.594	(1)
350.2	0.334	0.666	(1)
355.2	0.282	0.718	(1)
360.7	0.214	0.786	(1)
365.4	0.159	0.841	(1)
369.7	0.109	0.891	(1)
372.7	0.060	0.940	(1)
376.7	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.341 and at *T*/K = 308.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.	(1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 2,4,6-Trinitro-1-methylbenzene; $C_7H_5N_3O_6$; [118-96-7]

ORIGINAL MEASUREMENTS:

Kremann, R.

Monatsch. Chem. 1908, *29*, 863-890.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
351.2	1.000	0.000	(2)
347.2	0.896	0.104	(2)
343.2	0.828	0.172	(2)
345.2	0.787	0.213	1:1 Compound
351.7	0.709	0.291	1:1 Compound
355.2	0.669	0.331	1:1 Compound
358.2	0.610	0.390	1:1 Compound
360.2	0.551	0.449	1:1 Compound
360.7	0.505	0.495	1:1 Compound
360.7	0.483	0.517	1:1 Compound
360.2	0.459	0.541	1:1 Compound
359.7	0.444	0.556	1:1 Compound
358.0	0.406	0.594	1:1 Compound
355.2	0.371	0.629	1:1 Compound
352.2	0.342	0.658	1:1 Compound
350.7	0.322	0.678	1:1 Compound
350.2	0.297	0.707	(1)
360.2	0.204	0.796	(1)
365.2	0.159	0.841	(1)
369.2	0.102	0.898	(1)
371.7	0.072	0.928	(1)
374.7	0.041	0.959	(1)
376.7	0.000	1.000	(1)

Compiler: Phase diagram shows formation of a 1:1 molecular compound. Two eutectic points occur at about x_1 = 0.183 and T/K = 342.4 and at x_1 = 0.694 and T/K = 348.5.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 2,4-Dinitrophenol; $C_6H_4N_2O_5$; [51-28-5]

ORIGINAL MEASUREMENTS:

Kremann, R.; Hofmeier, F.

Monatsch. Chem. 1910, *31*, 201-202.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
384.2	1.000	0.000	(2)
382.2	0.970	0.030	(2)
380.2	0.928	0.072	(2)
377.2	0.872	0.128	(2)
374.2	0.845	0.155	(2)
371.2	0.797	0.203	(2)
369.2	0.755	0.245	(2)
366.2	0.718	0.282	(2)
363.2	0.677	0.323	(2)
360.2	0.641	0.359	(2)
355.2	0.595	0.405	(2)
350.2	0.558	0.442	(2)
347.2	0.507	0.493	(2)
340.2	0.475	0.525	(2)
335.2	0.446	0.554	(2)
337.2	0.415	0.585	(1)
341.2	0.376	0.624	(1)
346.2	0.336	0.664	(1)
351.2	0.286	0.714	(1)
356.2	0.235	0.765	(1)
363.2	0.163	0.837	(1)
369.2	0.103	0.897	(1)
374.2	0.043	0.957	(1)
376.2	0.000	1.000	(1)

Compiler: Eutectic point occurs at about x_1 = 0.562 and T/K = 334.8.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures prepared by weight. While the experimental details were not given in the paper, compiler speculates (based upon quantity of material used) that the sample was sealed in a glass container, temperature slowly varied, and the phase diagram determined by visually noting the temperature at which the last/first crystal of solid disappeared/appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 1-Chloro-4-nitrobenzene; $C_6H_4ClNO_2$; [100-00-5]

ORIGINAL MEASUREMENTS:

Rai, U.S.; Shekhar, H.

Thermochim. Acta 1991, *175*, 215-227.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the original paper, shows that the system is a simple eutectic system. The eutectic point occurs at circa x_1 = 0.44 and T/K = 316.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Thomas Backer & Co., Bombay, India, was purified by fractional recrystallization from ethanol.

(2) Purity not given, SD'S Lab-Chem. Industry, Bombay, India, purified by fractional recrystallization from ethanol.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.01 (Compiler).

COMPONENTS:

(1) Phenanthene; $C_{14}H_{10}$; [85-01-8]

(2) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]]

ORIGINAL MEASUREMENTS:

Burger, A.; Bryant, H.W.

J. Am. Chem. Soc. 1941, *63*, 1054-1057.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Experimentally determined phase diagram, which is depicted graphically in the in the original paper, shows phenanthrene + dibenzothiophene mixtures to form a simple eutectic system. The eutectic point occurs at circa x_2 = 0.52 and T/K = 349.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.01 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

ORIGINAL MEASUREMENTS:

Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; Eckert, C.A.
J. Chem. Eng. Data 1990, *35*, 446-449.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
429	1.00	0.00	(2)
425	0.95	0.05	(2)
423	0.90	0.10	(2)
420	0.85	0.15	(2)
416	0.80	0.20	(2)
412	0.75	0.25	(2)
409	0.70	0.30	(2)
405	0.65	0.35	(2)
400	0.60	0.40	(2)
397	0.55	0.45	(2)
390	0.50	0.50	(2)
383	0.45	0.55	(2)
377	0.40	0.60	(2)
370	0.35	0.65	(2)
362	0.30	0.70	(2)
356	0.25	0.75	(2)
357	0.20	0.80	(1)
361	0.15	0.85	(1)
365	0.10	0.90	(1)
369	0.05	0.95	(1)
372	0.00	1.00	(1)

Authors state that system exhibits simple eutectic behavior.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Samples were equilibrated in an apparatus similar to the one used by Ott and coworkers (see *J. Phys. Chem.* 1962, *66*, 1387). Temperature of the sample monitored with an Omega RTD probe inside a stainless steel tube that went down through the center of the pyrex tube. Samples heated above their melting point temperature, and time-temperature cooling curves were measured.

SOURCE AND PURITY OF MATERIALS:

(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized before use.

(2) 99.5 %, Aldrich Chemical Company, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.5.
x_1: ± 0.005 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) Benzoic Acid; $C_7H_6O_2$; [65-85-0]

ORIGINAL MEASUREMENTS:

Rai, U.S.; Shekhar, H.

Cryst. Res. Technol. 1990, *25*, 771-779.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase equilibrium data not given in cited paper. Authors report that the binary system has a single eutectic point which occurs at x_1 = 0.54 and T/K = 353.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures were prepared by weight. Melting and thaw point temperatures determined using a Toshiniwal Melting Point Apparatus equipped with a precision thermometer.

SOURCE AND PURITY OF MATERIALS:

(1) Purity unknown, Thomas Backer & Co., Bombay, India, was recrystallized from ethanol.

(2) Purity unknown, E. Merck, India, was recrystallized from boiling water.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.01 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) *trans*-Cinnamic Acid; $C_7H_6O_2$; [140-10-3]

ORIGINAL MEASUREMENTS:

Rai, U.S.; Shekhar, H.

Cryst. Res. Technol. 1990, *25*, 771-779.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase equilibrium data not given in cited paper. Authors report that the binary system has a single eutectic point which occurs at x_1 = 0.69 and T/K = 357.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures were prepared by weight. Melting and thaw point temperatures determined using a Toshiniwal Melting Point Apparatus equipped with a precision thermometer.

SOURCE AND PURITY OF MATERIALS:

(1) Purity unknown, Thomas Backer & Co., Bombay, India, was recrystallized from ethanol.

(2) Purity unknown, Sisco-Chem. Industry, India, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.01 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7]	Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; Eckert, C.A. *J. Chem. Eng. Data* <u>1990</u>, *35*, 446-449.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
432	1.00	0.00	(2)
423	0.90	0.10	(2)
416	0.80	0.20	(2)
410	0.70	0.30	(2)
404	0.60	0.40	(2)
398	0.50	0.50	(2)
390	0.40	0.60	(2)
381	0.30	0.70	(2)
368	0.20	0.80	(2)
367	0.10	0.90	(1)
370	0.00	1.00	(1)

Authors state that system exhibits simple eutectic behavior.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Samples were equilibrated in an apparatus similar to the one used by Ott and coworkers (see *J. Phys. Chem.* <u>1962</u>, *66*, 1387). Temperature of the sample monitored with an Omega RTD probe inside a stainless steel tube that went down through the center of the pyrex tube. Samples heated above their melting point temperature, and time-temperature cooling curves were measured.

SOURCE AND PURITY OF MATERIALS:

(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized before use.

(2) 99.5 %, Aldrich Chemical Company, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.5.
x_1: ± 0.005 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9]	Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; Eckert, C.A. *J. Chem. Eng. Data* <u>1990</u>, *35*, 446-449.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
472	1.00	0.00
466	0.90	0.10
457	0.80	0.20
454	0.70	0.30
451	0.60	0.40
450	0.50	0.50
449	0.40	0.60
447	0.30	0.70
440	0.20	0.80
426	0.10	0.90
372	0.00	1.00

Authors state that system exhibits behavior indicative of either compound formation or a solid solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Samples were equilibrated in an apparatus similar to the one used by Ott and coworkers (see *J. Phys. Chem.* <u>1962</u>, *66*, 1387). Temperature of the sample monitored with an Omega RTD probe inside a stainless steel tube that went down through the center of the pyrex tube. Samples heated above their melting point temperature, and time-temperature cooling curves were measured.

SOURCE AND PURITY OF MATERIALS:

(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized before use.

(2) 99.5 %, Aldrich Chemical Company, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.5.
x_1: ± 0.005 (Compiler).

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

(2) 6-Methyl-2,3,4-trinitrophenol; $C_7H_5N_3O_7$; [89793-90-8]

ORIGINAL MEASUREMENTS:

Efremov, N.N.; Fikhomirova, A.N.

J. Russ. Phys. Chem. Soc. 1927, *57*, 373-390.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase equilibrium data not given in cited paper. Authors report formation of a 1:1 phenanthrene - 6-methyl-2,3,4-trinitrophenol molecular compound. The two eutectic points occur at $x_1 = 0.176$ and $T/K = 358.8$ and at $x_1 = 0.825$ and $T/K = 357.4$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental details not given in paper.

determined using a Toshiniwal Melting Point Apparatus equipped with a precision thermometer.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.003 (Compiler).

1,10-PHENANTHROLINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

methanol + water
ethanol + water

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) 1,10-Phenanthroline; $C_{12}H_8N_2$; [5144-89-8] (2) Methanol; CH_4O; [67-56-1] (3) Water; H_2O; [7732-18-5]	Burgess, J.; Haines, R.I. *J. Chem. Eng. Data* 1978, *23*, 196-197.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$\phi_2^{(s)}$	$c_1/(\text{mol dm}^{-3})$
0.00	0.0149
0.05	0.0173
0.10	0.0207
0.15	0.0247
0.20	0.0280
0.25	0.0339

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: solubility of the solute expressed in terms of molarity. Equilibrium solid phase is probably a hydrated form of 1,10-phenanthroline, particularly in the water-rich binary solvent mixtures.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 298.2 nm. Attainment of equilibrium verified by several repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified, was recrystallized from aqueous-ethanol.

(2) Purity and chemical source not specified in paper.

(3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: ± 0.1 (Compiler).
$\phi_2^{(s)}$: ± 0.01 (Compiler).
c_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) 1,10-Phenanthroline; $C_{12}H_8N_2$; [5144-89-8]
(2) Methanol; CH_4O; [67-56-1]
(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sengupta, D.; Amalendu, P.; Lahiri, S.C.

J. Chem. Soc., Dalton Trans. 1983, 2685-2688.

VARIABLES:

T/K = 295, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]
t = 22.0 °C

$x_2^{(s)}$	c_1/(mol dm^{-3})
0.000	0.0169
0.047	0.0269
0.099	0.0591
0.159	0.1496
0.228	0.4491
0.307	1.1412
0.400	2.5072
0.508	5.1028
0.639	1.0528

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; c_1: solubility of the solute expressed in terms of molarity. Equilibrium solid phase is probably a hydrated form of 1,10-phenanthroline, particularly in the water-rich binary solvent mixtures.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures prepared volumetrically and solvent weight percentages calculated from known densities of the pure solvents at 295 K. Excess solute and solvent allowed to equilibrate for 24 hours in a Campbell solubility apparatus. Saturated solutions were filtered and withdrawn by inversion of the apparatus. Concentrations determined spectrophotometrically at 264 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent grade, E. Merck, was used as received from chemical supplier.

(2) Purity and chemical source not specified in paper.

(3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: ± 0.1 (Compiler).
$x_2^{(s)}$: ± 0.001 (Compiler).
c_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) 1,10-Phenanthroline; $C_{12}H_8N_2$; [5144-89-8]
(2) Ethanol; C_2H_6O; [64-17-5]
(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bhattacharyya, A.K.; Sengupta, D.; Lahiri, S.C.

Z. Phys. Chem., Leipzig 1984, *265*, 372-378.

VARIABLES:

T/K = 295, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 22.0 °C

$x_2^{(s)}$	c_1/(mol dm^{-3})
0.000	0.0170
0.033	0.0439
0.071	0.1040
0.117	0.3497
0.170	1.0117
0.235	2.2700
0.325	3.9585
0.418	6.8192
0.553	12.6205

[a] $x_2^{(s)}$: initial mole fraction of binary solvent mixture; c_1: solubility of the solute expressed in terms of molarity. Equilibrium solid phase is probably a hydrated form of 1,10-phenanthroline, particularly in the water-rich binary solvent mixtures.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures prepared volumetrically and solvent weight percentages calculated from known densities of the pure solvents at 295 K. Excess solute and solvent allowed to equilibrate for 24 hours in a Campbell solubility apparatus. Saturated solutions were filtered and withdrawn by inversion of the apparatus. Concentrations determined spectrophotometrically at 280 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent grade, E. Merck, was used as received from chemical supplier.

(2) Absolute, chemical supplier not specified in paper, was dried over calcium oxide and distilled before use.

(3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: ± 0.1 (Compiler).
$x_2^{(s)}$: ± 0.001 (Compiler).
c_1: ± 3 % (relative error, Compiler).

PHENOTHIAZINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

phenoxazine
thianthrene
phenoxanthiin
dibenzo[b,e][1,4]dioxine

J. Binary Solvent Mixtures

COMPONENTS:

(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2]

(2) Phenoxazine; $C_{12}H_9NO$; [135-67-1]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
429.9	429.1	1.000	0.000
427.3	415.3	0.941	0.059
424.3	413.0	0.871	0.129
416.7	413.2	0.744	0.256
415.2	412.9	0.735	0.265
415.8	413.1	0.689	0.311
430.1	413.6	0.483	0.517
438.1	413.0	0.360	0.640
449.5	416.9	0.176	0.824
452.0	421.5	0.118	0.882
457.6	456.8	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a partial series of solid solutions having compositions from circa $x_2 = 0.00$ to $x_2 = 0.22$ and from $x_2 = 0.93$ to $x_2 = 1.00$. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was sublimed and recrystallized from alcohol.

(2) Synthesized by the authors, was purified by sublimation and recrystallized from alcohol.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2]

(2) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
429.9	429.1	1.000	0.000
426.4	414.7	0.906	0.094
422.7	406.0	0.838	0.162
418.0	402.6	0.740	0.260
409.0	403.2	0.618	0.382
407.6	403.2	0.559	0.441
424.5	403.3	0.439	0.561
437.8	402.7	0.291	0.709
451.7	404.4	0.106	0.894
455.4	421.2	0.041	0.959
457.6	456.8	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a partial series of solid solutions having compositions from circa x_1 = 0.00 to x_1 = 0.20 and from x_1 = 0.89 to x_1 = 1.00. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was sublimed and recrystallized from alcohol.

(2) Purity and chemical source were not specified in paper, was purified by sublimation and recrystallization from acetone.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).

x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Phenoxanthiin; $C_{12}H_8OS$; [262-20-4]	Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
328.9	328.5	1.000	0.000
360.5	330.8	0.887	0.113
396.8	335.5	0.708	0.292
425.0	344.1	0.463	0.537
437.0	352.6	0.339	0.661
449.1	373.5	0.168	0.832
456.5	413.4	0.028	0.972
457.6	456.8	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a complete series of solid solutions. Melting points of binary mixtures lie between those of the two pure components. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.	(1) Purity and chemical source were not specified in paper, was sublimed and recrystallized from alcohol. (2) Synthesized by the authors, was purified by sublimation and recrystallized from alcohol.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2]

(2) Dibenzo[b,e][1,4]dioxin; $C_{12}H_8O_2$; [262-12-4]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
393.1	1.000	0.000	425.0	0.485	0.515
392.8	0.981	0.019	447.4	0.211	0.789
387.5	0.892	0.108	456.0	0.050	0.950
383.2	0.832	0.168	457.6	0.000	1.000
389.8	0.780	0.220			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was purified by sublimation and recrystallization from alcohol.

(2) Purity and chemical source not given, purified by recrystallization from alcohol and sublimed.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).

x_1: ± 0.002 (Compiler).

PHENOXANTHIIN SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

phenoxazine
thianthrene
phenothiazine
dibenzo[b,e][1,4]dioxin

J. Binary Solvent Mixtures

COMPONENTS:

(1) Phenoxanthiin; $C_{12}H_9OS$; [262-20-4]

(2) Phenoxazine; $C_{12}H_8NO$; [135-67-1]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
429.9	1.000	0.000	338.3	0.166	0.834
427.0	0.943	0.057	324.4	0.102	0.898
415.9	0.789	0.211	327.2	0.067	0.933
388.4	0.492	0.508	328.5	0.026	0.974
349.8	0.229	0.711	328.9	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by authors, and was purified by recrystallization from alcohol and sublimation.

(2) Synthesized by authors, and was purified by sublimation and recrystallized from alcohol.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenoxanthiin; $C_{12}H_8OS$; [262-20-4]

(2) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
429.9	1.000	0.000	357.4	0.189	0.811
426.8	0.900	0.100	337.2	0.100	0.900
415.3	0.699	0.301	326.1	0.070	0.930
399.5	0.513	0.487	328.3	0.046	0.954
378.7	0.308	0.692	328.9	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by the authors, was purified by sublimation and recrystallized from alcohol.

(2) Purity and chemical source not given, was purified by sublimation and recrystallization from acetone.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Phenoxanthiin; $C_{12}H_8OS$; [262-20-4] (2) Phenothiazine; $C_{12}H_9NS$; [92-84-2]	**ORIGINAL MEASUREMENTS:** Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
457.6	456.8	1.000	0.000
456.5	413.4	0.972	0.028
449.1	373.5	0.832	0.168
437.0	352.6	0.661	0.339
425.0	344.1	0.537	0.463
398.8	335.5	0.292	0.708
360.5	330.8	0.113	0.887
328.9	328.5	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a complete series of solid solutions. Melting points of binary mixtures lie between those of the two pure components. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.	**SOURCE AND PURITY OF MATERIALS:** (1) Synthesized by the authors, was purified by sublimation and recrystallized from alcohol. (2) Purity and chemical source not given in paper, was sublimed and recrystallized from alcohol.
	ESTIMATED ERRORS: *T*/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenoxanthiin; $C_{12}H_9OS$; [262-20-4]

(2) Dibenzo[b,e][1,4]dioxin; $C_{12}H_8O_2$; [262-12-4]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
393.1	1.000	0.000	335.8	0.218	0.782
390.9	0.943	0.057	320.4	0.096	0.904
380.1	0.739	0.261	325.5	0.052	0.948
367.6	0.561	0.439	327.1	0.000	1.000
348.2	0.337	0.663			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by authors, and was purified by recrystallization from alcohol and sublimation.

(2) Purity and chemical source not specified in paper, purified by sublimation and recrystallized from acetone.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).

x_1: ± 0.002 (Compiler).

PHENOXAZINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

phenothiazine
phenoxanthiin
thianthrene
dibenzo[b,e][1,4]dioxin

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenoxazine; $C_{12}H_9NO$; [135-67-1] (2) Phenothiazine; $C_{12}H_9NS$; [92-84-2]	Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
457.6	456.8	1.000	0.000
452.0	421.5	0.882	0.118
449.5	416.9	0.824	0.176
438.1	413.0	0.640	0.360
430.1	413.6	0.517	0.483
415.8	413.1	0.311	0.689
415.2	412.9	0.265	0.735
416.7	413.2	0.256	0.744
424.3	413.0	0.129	0.871
427.3	415.3	0.059	0.941
429.9	429.2	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a partial series of solid solutions having compositions from circa x_1 = 0.00 to x_1 = 0.22 and from x_1 = 0.93 to x_1 = 1.00. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.	(1) Synthesized by the authors, was purified by sublimation and recrystallized from alcohol. (2) Purity and chemical source were not specified in paper, was sublimed and recrystallized from alcohol.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Phenoxazine; $C_{12}H_9NO$; [135-67-1] (2) Phenoxanthiin; $C_{12}H_8OS$; [262-20-4]	**ORIGINAL MEASUREMENTS:** Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
328.9	1.000	0.000	349.8	0.771	0.229
328.5	0.974	0.026	388.4	0.508	0.492
327.2	0.933	0.067	415.9	0.211	0.789
324.4	0.898	0.102	427.0	0.057	0.943
338.8	0.834	0.166	429.9	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by authors, and was purified by recrystallization from alcohol and sublimation.
(2) Synthesized by authors, and was purified by sublimation and recrystallized from alcohol.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Phenoxazine; $C_{12}H_9NO$; [135-67-1] (2) Thianthrene; $C_{12}H_8S_2$; [92-85-3]	**ORIGINAL MEASUREMENTS:** Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
429.9	1.000	0.000	393.4	0.439	0.561
427.5	0.946	0.054	412.2	0.241	0.759
416.4	0.749	0.251	428.1	0.033	0.967
399.4	0.531	0.469	429.9	0.000	1.000
392.0	0.458	0.542			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by authors, and was purified by recrystallization from alcohol and sublimation.
(2) Purity and chemical source not given in paper, was purified by sublimation and repeated recrystallizations from acetone.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Phenoxazine; $C_{12}H_9NO$; [135-67-1]

(2) Dibenzo[b,e][1,4]dioxin; $C_{12}H_8O_2$; [262-12-4]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
393.1	392.6	1.000	0.000
390.4	378.4	0.903	0.097
387.5	373.6	0.835	0.165
385.0	369.2	0.774	0.226
381.1	363.3	0.703	0.297
367.1	363.5	0.648	0.352
374.4	363.4	0.608	0.392
396.4	363.0	0.486	0.514
413.3	364.7	0.291	0.709
418.5	371.4	0.208	0.792
423.8	387.3	0.121	0.879
429.9	429.2	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a partial series of solid solutions having compositions from circa x_1 = 0.00 to x_1 = 0.30 and from x_1 = 0.70 to x_1 = 1.00. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by the authors, was purified by sublimation and recrystallized from alcohol.

(2) Purity and chemical source were not specified in paper, was sublimed and recrystallized from acetone.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).

x_1: ± 0.002 (Compiler).

PYRENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
n-octadecane
cyclohexane
methylcyclohexane
cyclooctane
2,2,4-trimethylpentane
t-butylcyclohexane

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,2-dimethylbenzene
1,3-dimethylbenzene
1,4-dimethylbenzene
chrysene
naphthalene

D. Esters

ethyl ethanoate
butyl ethanoate
ethyl butyrate

E. Ethers

1,1-oxybisbutane
1,4-dioxane

F. Haloalkanes and Haloaromatic Hydrocarbons

tetrachloromethane
1,2-dichloroethane
1-chlorobutane
1,4-dichlorobutane
octafluoronaphthalene

G. Alcohols

methanol
ethanol
1-propanol
2-propanol
1-butanol
2-butanol
1-pentanol
2-methyl-1-propanol
3-methyl-1-butanol
1-octanol

cyclopentanol
1-hydroxy-2-methylbenzene

H. Ketones

2-propanone

I. Miscellaneous Pure Solvents

pyridine
dimethyl sulfoxide
acetonitrile
1,3-dinitrobenzene
1,4-dinitrobenzene
1,3,5-trinitrobenzene
1,2,3,5-tetranitrobenzene
2,4-dinitromethylbenzene
2,4-dinitrophenol
2,4,6-trinitromethylbenzene
2,4,6-trinitromethoxybenzene
2,4,6-trinitroaniline
2-chloro-1,3,5-trinitrobenzene
3-methyl-2,4,6-trinitrophenol

J. Binary Solvent Mixtures

n-hexane + 1-propanol
n-heptane + 1-propanol
n-octane + 1-propanol
cyclohexane + 1-propanol
methylcyclohexane + 1-propanol
2,2,4-trimethylpentane + 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

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
26.0	0.9915	0.00852

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
26.0	0.9890	0.01101

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	$c_1/(\text{mol dm}^{-3})$
20.0	0.0120

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifugation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming that the dilute solution behavior extrapolates up to saturation point.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/° C$	x_2	x_1
26.0	0.9862	0.01379

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) n-Octadecane; $C_{18}H_{38}$; [593-45-3]	Djordjevic, N.M. *Thermochim. Acta* 1991, *177*, 109-118.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
407.0	0.3939	0.6061	411.2	0.2388	0.7612
409.1	0.3095	0.6905	412.5	0.1765	0.8235
409.7	0.2972	0.7028	417.2	0.1014	0.8986
410.5	0.2671	0.7329	419.0	0.0498	0.9502

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter.

Mixtures (1.5 - 2.0 mg) of known concentration were weighed into aluminum pans, which were then crimped to preclude sample loss during the heating process. Solubilities determined by measuring melting points of binary mixtures using a Perkin-Elmer DSC-2 differential scanning calorimeter and scan rate of 5 K/min.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (compiler).
x_1: ± 0.0003 (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1987, *32*, 60-62.
VARIABLES:	**PREPARED BY:**
T/K = 299	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
26.0	0.9891	0.01089

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	**ORIGINAL MEASUREMENTS:** McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 3854-3857.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
295.0	0.9916	0.0084
303.7	0.9871	0.0129
316.2	0.9799	0.0201
322.3	0.9749	0.0251

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.

(2) Purity, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	**ORIGINAL MEASUREMENTS:** Carre, O.R.; Phillips, D.J.; Brennecke, J.F. *Ind. Eng. Chem. Res.* 1994, *33*, 1355-1362.
VARIABLES: T/K = *Circa* 294 (Ambient Room)	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9886	0.0114

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) HPLC Grade, 99+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 2.4 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

ORIGINAL MEASUREMENTS:

Wallach, J.R.; Tucker, S.A.; Oswalt, B.M.; Murral, D.J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9870	0.0130

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 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 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Cyclooctane; C_8H_{16}; [292-64-8]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9804	0.01956

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 60-62.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9928	0.00721

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

ORIGINAL MEASUREMENTS:

Wallach, J.R.; Tucker, S.A.; Oswalt, B.M.; Murral, D.J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9841	0.0159

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *16*, 179-187.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
26.0	0.9368	0.06316

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.6	0.9266	0.0734	357.8	0.6986	0.3014
331.8	0.8494	0.1506			
340.0	0.8104	0.1896			
349.4	0.7559	0.2441			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Rutgerswerke A.G., Germany, was passed over an alumina column with benzene as eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.9433	0.0567

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared containers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not given, was recrystallized several times from toluene and ethanol to give a melting temperature of 150.5-150.9 °C.

(2) 99 %, Urxovy Zavody, Czech., was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, *33*, 1355-1362.

VARIABLES:

T/K = *Circa* 294 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9335	0.0665

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) ACS Grade, 99+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9322	0.06785

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,2-Dimethylbenzene; C_8H_{10}; [95-47-6]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9239	0.07611

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 98+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9295	0.07055

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9317	0.06831

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Chrysene; $C_{18}H_{12}$; [218-01-9]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669. (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
528.2	1.000	0.000	(2)
517.7	0.897	0.103	(2)
506.7	0.782	0.218	(2)
496.2	0.686	0.314	(2)
487.2	0.604	0.396	(2)
473.2	0.495	0.505	(2)
458.7	0.398	0.602	(2)
441.2	0.303	0.697	(2)
420.6	0.210	0.790	(2)
415.4	0.187	0.813	(2)
408.2	0.165	0.835	Eutectic
410.2	0.136	0.864	(1)
413.7	0.099	0.901	(1)
423.2	0.000	1.000	(1)

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Naphthalene; $C_{10}H_8$; [91-20-3]

ORIGINAL MEASUREMENTS:

Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M.
Bull. Chem. Soc. Japan 1985, *58*, 3643-3644.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the original paper, shows that the system is a simple eutectic system. The eutectic point occurs at circa x_1 = 0.22 and T/K = 335.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical grade, Katayama Chemicals, Japan, was used as received.

(2) Reagent grade, Katayama Chemicals, Japan, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.02 (Compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9575	0.04251

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.9 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9407	0.05932

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Ethyl butyrate; $C_6H_{12}O_2$; [105-54-4]

ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, *33*, 1355-1362.

VARIABLES:

T/K = *Circa* 294 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
21.0	0.9460	0.0540

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 6.0 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

Wallach, J.R.; Tucker, S.A.; Oswalt, B.M.; Murral, D.J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1989, *34*, 70-73.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9702	0.0298

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.791

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9648	0.03520

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 2485-2488.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
314.2	0.9298	0.0702
331.6	0.8811	0.1189
342.2	0.8361	0.1639
352.4	0.7810	0.2190

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.

(2) AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	**ORIGINAL MEASUREMENTS:** Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. *Phys. Chem. Liq.*, in press.
VARIABLES: T/K = 299	**PREPARED BY:** W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9577	0.04229

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.	**SOURCE AND PURITY OF MATERIALS:** (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol. (2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** T/K: ± 0.05. x_1: ± 1.3 % (relative error).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	**ORIGINAL MEASUREMENTS:** Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. *Phys. Chem. Liq.*, in press.
VARIABLES: T/K = 299	**PREPARED BY:** W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9125	0.08746

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.	**SOURCE AND PURITY OF MATERIALS:** (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol. (2) 99+ %, Aldrich Chemical Company, anhydrous, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** T/K: ± 0.05. x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1-Chlorobutane; C_4H_9Cl; [109-69-3]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9391	0.06094

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.

J. Chem. Soc., Faraday Trans. 1990, *86*, 2197-2201.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.8903	0.1097

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Octafluoronaphthalene; $C_{10}F_8$; [313-72-4]

ORIGINAL MEASUREMENTS:

Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M.
Bull. Chem. Soc. Japan 1985, *58*, 3643-3644.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase diagram, given in the original paper, shows formation of a 1:1 pyrene - octafluoronaphthalene molecular compound having a melting point of circa 528.2 K. Two eutectic points occur at about x_2 = 0.07 and T/K = 422.2, and at about x_2 = 0.95 and T/K = 321.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical grade, Katayama Chemicals, Japan, was used as received.

(2) Reagent grade, Tokyo Chemical Company, Japan, was recrystallized from methanol before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.02 (Compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.0673

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9985	0.00149

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.9971	0.00288

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not given, was recrystallized several times from toluene and ethanol to give a melting temperature of 150.5-150.9 °C.

(2) Commercial sample, purity and source not specified, was dehydrated and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°$ C	x_2	x_1
26.0	0.9968	0.00317

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) Absolute, Aaper Alcohol and Chemical Company, Shelbyville, Kentucky, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°$ C	x_2	x_1
26.0	0.9957	0.00426

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [67-63-0]	Zvaigzne, A.I.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1993, *38*, 393-395.
VARIABLES:	**PREPARED BY:**
T/K = 299	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9971	0.00290

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. *Phys. Chem. Liq.*, in press.
VARIABLES:	**PREPARED BY:**
T/K = 299	W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9938	0.00622

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.8 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9957	0.00433

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, anhydrous, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9907	0.00926

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9968	0.00319

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, anhydrous, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9945	0.00546

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, anhydrous, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9790	0.02097

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Aldrich Chemical Company, anhydrous, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.1399

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

$T/K = 299$

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
26.0	0.9901	0.00994

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 1-Hydroxy-2-methylbenzene; C_7H_8O; [95-48-7]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

$T/K = 296$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	$c_1/(\mathrm{mol\ dm^{-3}})$
23.0	0.218

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
20.0	0.9716	0.0284

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not given, was recrystallized several times from toluene and ethanol to give a melting temperature of 150.5-150.9 °C.

(2) Commercial sample, purity and source not specified, was dehydrated and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.

Phys. Chem. Liq., in press.

VARIABLES:

T/K = 299

PREPARED BY:

W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/° C	x_2	x_1
26.0	0.9639	0.03612

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Krezewki, R.; Smutek, M.

Collection Czech. Chem. Commun. 1967, *32*, 1258-1259.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
20.0	0.9127	0.0873

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, source not given, was recrystallized several times from toluene and ethanol to give a melting temperature of 150.5-150.9 °C.
(2) Purity not given, Urxovy Zavody, Czech., treated with potassium permanganate, dried over potassium hydroxide and then distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$c_1/(\text{mol dm}^{-3})$
23.0	0.396

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Acetonitrile; C_2H_3N; [75-05-8]	**ORIGINAL MEASUREMENTS:** Carre, O.R.; Phillips, D.J.; Brennecke, J.F. *Ind. Eng. Chem. Res.* 1994, *33*, 1355-1362.
VARIABLES: T/K = *Circa* 294 (Ambient Room)	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9943	0.00574

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 0.6 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
363.2	1.000	0.000	365.0	0.554	0.446
358.2	0.913	0.087	365.7	0.499	0.501
354.2	0.854	0.146	366.0	0.496	0.504
357.2	0.831	0.169	365.2	0.476	0.524
359.7	0.790	0.210	364.2	0.449	0.551
360.2	0.762	0.238	376.2	0.430	0.570
362.2	0.702	0.298	367.2	0.429	0.571
362.5	0.665	0.335	376.2	0.391	0.609
362.2	0.621	0.379	384.2	0.341	0.659
363.7	0.586	0.414	395.7	0.277	0.723
364.7	0.563	0.437	423.2	0.000	1.000

Author reports formation of a 1:1 pyrene - 1,3-dinitrobenzene orangish-yellow molecular compound having a melting point temperature of 365.9 K, and a second 1:2 pyrene - 1,3-dinitrobenzene yellow compound with melting point of 362.5 K. Three eutectic points occur at x_1 = 0.130 and T/K = 352.2, x_1 = 0.366 and T/K = 361.2, and at x_1 = 0.565 and T/K = 362.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,4-Dinitrobenzene; $C_6H_4N_2O_4$; [100-25-4]	**ORIGINAL MEASUREMENTS:** Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
446.7	1.000	0.000	386.2	0.413	0.587
432.2	0.818	0.182	386.2	0.402	0.598
422.7	0.715	0.285	385.2	0.395	0.605
415.2	0.666	0.334	382.7	0.360	0.640
414.2	0.622	0.378	384.5	0.349	0.651
403.2	0.554	0.446	384.2	0.340	0.660
400.7	0.536	0.464	388.2	0.332	0.668
389.2	0.484	0.516	402.2	0.284	0.716
388.2	0.460	0.540	395.5	0.260	0.740
387.2	0.435	0.565	417.2	0.066	0.934
386.7	0.419	0.581	423.2	0.000	1.000

Author reports formation of a 1:1 pyrene - 1,4-dinitrobenzene bright red molecular compound having an incongruent melting point temperature. A eutectic point occurs at x_1 = 0.637 and T/K = 380.7, and a pertectic point occurs at x_1 = 0.520 and T/K = 387.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details given in paper.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,3,5-Trinitrobenzene; $C_6H_3N_3O_6$; [99-35-4]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
396.2	1.000	0.000	(2)
420.2	0.950	0.050	1:1 Compound
478.2	0.828	0.172	1:1 Compound
478.2	0.826	0.174	1:1 Compound
500.2	0.740	0.260	1:1 Commpound
514.7	0.627	0.373	1:1 Compound
518.7	0.514	0.486	1:1 Compound
517.2	0.447	0.553	1:1 Compound
508.7	0.321	0.679	1:1 Compound
482.5	0.222	0.778	1:1 Compound
466.7	0.160	0.840	1:1 Compound
439.2	0.125	0.875	1:1 Compound
423.2	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 1,3,5-trinitrobenzene reddish-orange molecular compound having a melting point temperature of 518.7 K. Two eutectic points occur at $x_1 = 0.020$ and $T/K = 389.2$, and at $x_1 = 0.900$ and $T/K = 414.7$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,2,3,5-Tetranitrobenzene; $C_6H_2N_4O_8$; [3698-53-1]	**ORIGINAL MEASUREMENTS:** Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
399.2	1.000	0.000	(2)
398.2	0.904	0.096	1:1 Compound
435.2	0.661	0.339	1:1 Compound
439.7	0.594	0.406	1:1 Compound
441.2	0.510	0.490	1:1 Compound
441.2	0.503	0.497	1:1 Compound
435.2	0.406	0.594	1:1 Compound
431.2	0.380	0.620	1:1 Compound
414.2	0.251	0.749	1:1 Compound
400.2	0.205	0.795	1:1 Compound
403.2	0.162	0.838	(1)
420.2	0.042	0.958	(1)
423.2	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 1,2,3,5-tetranitrobenzene dark red molecular compound having a melting point temperature of 441.7 K. Two eutectic points occur at x_1 = 0.085 and T/K = 395.2, and at x_1 = 0.810 and T/K = 398.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details given in paper.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,4-Dinitromethylbenzene; $C_7H_6N_2O_4$; [121-14-2]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
344.2	1.000	0.000	(2)
333.7	0.823	0.178	(2)
337.2	0.788	0.212	1:1 Compound
342.2	0.758	0.242	1:1 Compound
355.2	0.689	0.311	1:1 Compound
358.7	0.641	0.359	1:1 Compound
363.5	0.583	0.417	1:1 Compound
365.2	0.519	0.481	1:1 Compound
365.7	0.506	0.494	1:1 Compound
364.0	0.449	0.551	(1)
379.7	0.382	0.618	(1)
394.2	0.270	0.730	(1)
397.7	0.242	0.758	(1)
415.7	0.098	0.902	(1)
423.7	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 2,4-dinitromethylbenzene yellow molecular compound having a melting point temperature of 365.7 K. Two eutectic points occur at x_1 = 0.197 and T/K = 330.7, and at x_1 = 0.544 and T/K = 362.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2,4-Dinitrophenol; $C_6H_4N_2O_5$; [51-28-5]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

J. Chem. Soc. Japan 1940, *15*, 259-270.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
386.7	1.000	0.000	(2)
382.2	0.924	0.076	(2)
386.2	0.805	0.195	1:1 Compound
416.2	0.610	0.390	1:1 Compound
419.2	0.530	0.470	1:1 Compound
419.7	0.506	0.494	1:1 Compound
419.2	0.456	0.544	1:1 Compound
418.2	0.448	0.552	1:1 Compound
407.7	0.335	0.665	1:1 Compound
405.7	0.180	0.820	(1)
416.2	0.077	0.923	(1)
423.2	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 2,4-dinitrophenol reddish-orange molecular compound having a melting point temperature of 419.5 K. Two eutectic points occur at x_1 = 0.156 and T/K = 374.2, and at x_1 = 0.736 and T/K = 393.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,4,6-Trinitromethylbenzene; $C_7H_5N_3O_6$; [118-96-7]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
354.7	1.000	0.000	(2)
354.2	0.944	0.056	1:1 Compound
375.2	0.890	0.110	1:1 Compound
400.2	0.835	0.165	1:1 Compound
408.7	0.790	0.210	1:1 Compound
417.2	0.741	0.259	1:1 Compound
426.7	0.670	0.330	1:1 Compound
436.2	0.550	0.450	1:1 Compound
437.7	0.482	0.518	1:1 Compound
436.7	0.431	0.569	1:1 Compound
427.2	0.315	0.685	1:1 Compound
415.7	0.239	0.761	1:1 Compound
405.2	0.156	0.844	(2)
421.2	0.029	0.971	(2)
423.2	0.000	1.000	(2)

Author reports formation of a 1:1 pyrene - 2,4,6-trinitromethylbenzene orange molecular compound having a melting point temperature of 437.7 K. Two eutectic points occur at x_1 = 0.048 and T/K = 348.2, and at x_1 = 0.812 and T/K = 399.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,4,6-Trinitromethoxybenzene; $C_7H_5N_3O_7$; [606-35-9]	Shinomiya, C. *J. Chem. Soc. Japan* <u>1940</u>, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
341.2	1.000	0.000	(2)
356.2	0.867	0.133	1:1 Compound
365.2	0.796	0.204	1:1 Compound
365.7	0.782	0.218	1:1 Compound
373.2	0.660	0.340	1:1 Compound
376.2	0.569	0.431	1:1 Compound
377.2	0.532	0.468	1:1 Compound
377.7	0.471	0.529	1:1 Compound
377.7	0.376	0.624	(1)
385.2	0.346	0.654	(1)
401.2	0.222	0.778	(1)
413.7	0.125	0.875	(1)
423.2	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 2,4,6-trinitromethoxybenzene yellowish-orange compound having a melting point temperature of 377.7 K. Two eutectic points occur at x_1 = 0.030 and T/K = 333.7, and at x_1 = 0.605 and T/K = 371.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,4,6-Trinitroaniline; $C_6H_4N_3O_6$; [489-98-5]	**ORIGINAL MEASUREMENTS:** Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
461.7	1.000	0.000	(2)
468.7	0.834	0.166	1:1 Compound
486.7	0.731	0.269	1:1 Compound
504.2	0.614	0.386	1:1 Compound
509.2	0.497	0.503	1:1 Compound
508.7	0.480	0.520	1:1 Compound
505.5	0.377	0.623	1:1 Compound
501.7	0.346	0.654	1:1 Compound
486.2	0.262	0.738	1:1 Compound
472.2	0.186	0.814	1:1 Compound
447.2	0.118	0.882	1:1 Compound
442.2	0.085	0.915	1:1 Compound
418.2	0.053	0.947	(1)
423.2	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 2,4,6-trinitroaniline brown molecular compound having a melting point temperature of 509.2 K. Two eutectic points occur at x_1 = 0.122 and *T*/K = 453.7, and at x_1 = 0.920 and *T*/K = 412.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details given in paper.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper.
	ESTIMATED ERRORS: *T*/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Chloro-1,3,5-trinitrobenzene; $C_6H_2ClN_3O_6$; [88-88-0]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
356.2	1.000	0.000
352.2	0.913	0.087
401.7	0.776	0.224
418.2	0.700	0.300
425.2	0.570	0.430
426.7	0.509	0.491
423.2	0.426	0.574
409.2	0.301	0.699
407.7	0.188	0.712
417.0	0.090	0.910
423.2	0.000	1.000

Author reports formation of a 1:1 pyrene - 2-chloro-1,3,5-trinitrobenzene brownish-red compound having a melting point of 427.2 K. Two eutectic points occur at x_1 = 0.080 and T/K = 346.7, and at x_1 = 0.770 and T/K = 398.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Chloro-1,3,5-trinitrobenzene; $C_6H_2ClN_3O_6$; [88-88-0]	**ORIGINAL MEASUREMENTS:** Krajewska, A.; Wasilewska, K. *Thermochim. Acta* 1981, *44*, 117-120.
VARIABLES:	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

Authors report that the binary system exhibits a fairly simple phase diagram. A 1:1 pyrene - 2-chloro-1,3,5-trinitrobenzene molecular compound with melting point of $T/K = 429$, and an incongruently melting 3:2 pyrene - 2-chloro-1,3,5-trinitrobenzene molecular compound were observed.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Differential scanning calorimeter and thermostated light microscope. Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric and microscopic techniques.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.1 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Chloro-1,3,5-trinitrobenzene; $C_6H_2ClN_3O_6$; [88-88-0]	**ORIGINAL MEASUREMENTS:** Bando, M.; Matsunaga, Y. *Bull. Chem. Soc. Japan* 1976, *49*, 3345-3346.
VARIABLES:	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

Authors report formation of a 1:1 pyrene - 2-chloro-1,3,5-trinitrobenzene molecular compound having a melting point of 427.2 K. An eutectic point occurs at $x_1 = 0.120$ and $T/K = 348.2$. Four incongruently melting pyrene - 2-chloro-1,3,5-trinitrobenzene compounds with 4:3, 2:1, 3:1 and 4:1 stoichoimetries were also reported to exist.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Differential scanning calorimeter. Binary mixtures were prepared by weight. Melting points and transition temperatures determined using a differential scanning calorimeter An experimental phase diagram is given in the original paper.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper. (2) Purity and chemical source were not specified in paper. **ESTIMATED ERRORS:** T/K: precision ± 0.1 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 3-Methyl-2,4,6-trinitrophenol; $C_7H_5N_3O_7$; [602-99-3]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
381.7	1.000	0.000	(2)
405.7	0.847	0.153	1:1 Compound
420.2	0.754	0.246	1:1 Compound
426.7	0.699	0.301	1:1 Compound
434.2	0.578	0.422	1:1 Compound
436.2	0.529	0.471	1:1 Compound
434.2	0.449	0.551	1:1 Compound
425.2	0.290	0.710	1:1 Compound
421.2	0.235	0.765	1:1 Compound
413.2	0.109	0.891	(1)
423.2	0.000	1.000	(1)

Author reports formation of a 1:1 pyrene - 3-methyl-2,4,6-trinitrophenol reddish-brown compound having a melting point of 436.2 K. Two eutectic points occur at x_1 = 0.075 and T/K = 374.2, and at x_1 = 0.848 and T/K = 408.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details given 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 ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) n-Hexane; C_6H_{14}; [110-54-3] (3) 1-Propanol; C_3H_8O; [71-23-8]	Zvaigzne, A.I.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1993, *38*, 393-395.
VARIABLES:	**PREPARED BY:**
T/K = 299, Solvent composition	W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00857
0.1727	0.1711	0.00944
0.3063	0.3036	0.00895
0.5431	0.5388	0.00787
0.6400	0.6353	0.00728
0.7258	0.7209	0.00669
0.8734	0.8686	0.00545
0.9338	0.9292	0.00490
1.0000	0.9957	0.00426

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01102
0.1927	0.1905	0.01154
0.3280	0.3244	0.01089
0.5599	0.5548	0.00916
0.6656	0.6602	0.00814
0.7383	0.7329	0.00734
0.8810	0.8760	0.00568
0.9416	0.9369	0.00495
1.0000	0.9957	0.00426

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01372
0.1959	0.1932	0.01389
0.3597	0.3552	0.01261
0.5930	0.5869	0.01022
0.6798	0.6736	0.00910
0.7584	0.7523	0.00800
0.8873	0.8819	0.00612
0.9504	0.9456	0.00507
1.0000	0.9957	0.00426

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01100
0.1513	0.1495	0.01192
0.2741	0.2710	0.01141
0.4938	0.4890	0.00969
0.5957	0.5905	0.00876
0.6894	0.6841	0.00765
0.8750	0.8700	0.00573
0.9251	0.9205	0.00501
1.0000	0.9957	0.00426

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01292
0.1734	0.1711	0.01336
0.2997	0.2959	0.01271
0.5273	0.5218	0.01045
0.6238	0.6181	0.00921
0.7164	0.7107	0.00798
0.8672	0.8620	0.00599
0.9384	0.9337	0.00499
1.0000	0.9957	0.00426

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00720
0.2131	0.2115	0.00738
0.3581	0.3555	0.00721
0.5925	0.5886	0.00659
0.6783	0.6741	0.00624
0.7710	0.7665	0.00584
0.8887	0.8842	0.00511
0.9421	0.9377	0.00472
1.0000	0.9957	0.00426

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00857
0.1676	0.1661	0.00867
0.2966	0.2942	0.00825
0.5251	0.5214	0.00700
0.6303	0.6264	0.00619
0.7199	0.7160	0.00547
0.8651	0.8615	0.00412
0.9301	0.9268	0.00352
1.0000	0.9971	0.00290

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

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(2) 99+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01102
0.1872	0.1851	0.01117
0.3336	0.3302	0.01029
0.5561	0.5515	0.00830
0.6558	0.6511	0.00724
0.7436	0.7390	0.00618
0.8890	0.8852	0.00430
0.9390	0.9356	0.00367
1.0000	0.9971	0.00290

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

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(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

$T/K = 299$, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

$t = 26.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01372
0.1971	0.1944	0.01350
0.3555	0.3512	0.01210
0.5829	0.5774	0.00940
0.6836	0.6782	0.00796
0.7639	0.7588	0.00673
0.9006	0.8965	0.00451
0.9459	0.9423	0.00377
1.0000	0.9971	0.00290

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01100
0.1496	0.1479	0.01133
0.2625	0.2597	0.01082
0.4936	0.4893	0.00875
0.5936	0.5891	0.00764
0.6755	0.6710	0.00670
0.8559	0.8520	0.00451
0.9212	0.9177	0.00376
1.0000	0.9971	0.00290

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

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METHOD: APPARATUS/PROCEDURE

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(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01292
0.1691	0.1669	0.01325
0.2953	0.2917	0.01221
0.5220	0.5170	0.00960
0.6240	0.6189	0.00819
0.7238	0.7189	0.00673
0.8660	0.8619	0.00469
0.9336	0.9301	0.00374
1.0000	0.9971	0.00290

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

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METHOD: APPARATUS/PROCEDURE

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Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 393-395.

VARIABLES:

T/K = 299, Solvent composition

PREPARED BY:

W.E. Acree, Jr. and A.I. Zvaigzne

EXPERIMENTAL VALUES[a]

t = 26.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00720
0.1987	0.1972	0.00746
0.3622	0.3597	0.00690
0.5803	0.5769	0.00592
0.6848	0.6812	0.00532
0.7661	0.7624	0.00478
0.8908	0.8874	0.00380
0.9434	0.9402	0.00336
1.0000	0.9971	0.00290

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

THIANTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
cyclohexane
methylcyclohexane
cyclooctane
2,2,4-trimethylpentane

B. Alkenes

C. Aromatic Hydrocarbons

phenanthrene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

phenothiazine
phenoxanthiin
phenoxazine

J. Binary Solvent Mixtures

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9968	0.00320

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9965	0.00346

AUXILIARY INFORMATION \

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS: (1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) n-Octane; C_8H_{18}; [111-65-9]	**ORIGINAL MEASUREMENTS:** Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I. *Phys. Chem. Liq.* 1990, *21*, 45-49.
VARIABLES: T/K = 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.9961	0.00392

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.	**SOURCE AND PURITY OF MATERIALS:** (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol. (2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** T/K: ± 0.05. x_1: ± 1 % (relative error).

COMPONENTS: (1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Cyclohexane; C_6H_{12}; [110-82-7]	**ORIGINAL MEASUREMENTS:** Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I. *Phys. Chem. Liq.* 1990, *21*, 45-49.
VARIABLES: T/K = 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.9941	0.00587

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.	**SOURCE AND PURITY OF MATERIALS:** (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol. (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** T/K: ± 0.05. x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t/° C	x_2	x_1
25.0	0.9937	0.00631

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

(2) Cyclooctane; C_8H_{16}; [292-64-8]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.

Phys. Chem. Liq. 1990, *21*, 45-49.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t/° C	x_2	x_1
25.0	0.9877	0.01232

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.

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(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I. *Phys. Chem. Liq.* 1990, *21*, 45-49.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t/° C	x_2	x_1
25.0	0.9973	0.00273

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol. (2) HPLC Grade, 99.7 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** *T*/K: ± 0.05. x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Phenanthrene; $C_{14}H_{10}$; [85-01-8]	Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; Eckert, C.A. *J. Chem. Eng. Data* <u>1990</u>, *35*, 446-449.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	Solid Phase
372	1.00	0.00	(2)
369	0.95	0.05	(2)
365	0.90	0.10	(2)
361	0.85	0.15	(2)
357	0.80	0.20	(2)
356	0.75	0.25	(1)
362	0.70	0.30	(1)
370	0.65	0.35	(1)
377	0.60	0.40	(1)
383	0.55	0.45	(1)
390	0.50	0.50	(1)
397	0.45	0.55	(1)
400	0.40	0.60	(1)
405	0.35	0.65	(1)
409	0.30	0.70	(1)
412	0.25	0.75	(1)
416	0.20	0.80	(1)
420	0.15	0.85	(1)
423	0.10	0.90	(1)
425	0.05	0.95	(1)
429	0.00	1.00	(1)

Authors report that system exhibits simple eutectic behavior.

Compiler: Eutectic point occurs at about x_1 = 0.24 and *T*/K = 353.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Samples were equilibrated in an apparatus similar to the one used by Ott and coworkers (see *J. Phys. Chem.* <u>1962</u>, *66*, 1387). Temperature of the sample monitored with an Omega RTD probe inside a stainless steel tube that went down through the center of the pyrex tube. Samples heated above their melting point temperature, and time-temperature cooling curves were measured.	(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized before use. (2) 99.5 %, Aldrich Chemical Company, was recrystallized before use. **ESTIMATED ERRORS:** *T*/K: precision ± 0.5. x_1: ± 0.005 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Phenothiazine; $C_{12}H_9NS$; [92-84-2]	Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
457.6	456.8	1.000	0.000
455.4	421.2	0.959	0.041
451.7	404.4	0.894	0.106
437.8	402.7	0.709	0.291
424.5	403.3	0.561	0.439
407.6	403.2	0.441	0.559
409.0	403.2	0.382	0.618
418.0	402.6	0.260	0.740
422.7	406.0	0.162	0.838
426.4	414.7	0.094	0.906
429.9	429.1	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a partial series of solid solutions having compositions from circa x_2 = 0.00 to x_2 = 0.20 and from x_2 = 0.89 to x_2 = 1.00. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was purified by sublimation and recrystallization from acetone.
(2) Purity and chemical source were not specified in paper, was sublimed and recrystallized from alcohol.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

(2) Phenoxanthiin; $C_{12}H_8OS$; [262-20-4]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
328.9	1.000	0.000	378.7	0.692	0.308
328.3	0.954	0.046	399.5	0.487	0.513
326.1	0.930	0.070	415.3	0.301	0.699
337.2	0.900	0.100	426.8	0.100	0.900
357.4	0.811	0.189	429.9	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified, was purified by sublimation and recrystallized from acetone.

(2) Synthesized by authors, was purified by sublimation and recrystallized from alcohol.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]

(2) Phenoxazine; $C_{12}H_9NO$; [135-67-1]

ORIGINAL MEASUREMENTS:

Cullinane, N.M.; Rees, W.T.

Trans. Faraday Soc. 1940, *36*, 506-514.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
429.9	1.000	0.000	399.4	0.469	0.531
428.1	0.967	0.033	416.4	0.251	0.749
412.2	0.659	0.341	427.5	0.054	0.946
393.4	0.561	0.439	429.9	0.000	1.000
392.0	0.542	0.458			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was purified by sublimation and recrystallization from acetone.

(2) Synthesized by authors, and was purified by recrystallization from alcohol and sublimation.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

THIOXANTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
1,2,3,4-tetrahydronaphthalene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Thioxanthene; $C_{13}H_{10}S$; [261-31-4]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
318.3	0.9697	0.0303	354.8	0.8665	0.1335
331.8	0.9483	0.0517	368.5	0.7883	0.2117
338.5	0.9329	0.0671			
349.7	0.8916	0.1084			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Thioxanthene; $C_{13}H_{10}S$; [261-31-4]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.5	0.9648	0.0352	343.9	0.8721	0.1279
321.1	0.9456	0.0544	353.3	0.8090	0.1910
328.1	0.9297	0.0703			
337.8	0.8971	0.1029			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, gift from Dr. E. J. Esienbraum, Oklahoma State University, USA, was recrystallized from toluene.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Thioxanthene; $C_{13}H_{10}S$; [261-31-4]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
319.1	0.9028	0.0972	347.7	0.7472	0.2528
329.7	0.8611	0.1389	351.9	0.6999	0.3001
341.5	0.7999	0.2001			
343.9	0.7730	0.2270			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Thioxanthene; $C_{13}H_{10}S$; [261-31-4]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.2	0.9131	0.0869	344.5	0.7533	0.2467
317.3	0.8879	0.1121	352.0	0.6936	0.3064
328.8	0.8401	0.1599			
337.3	0.7956	0.2044			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, gift from Dr. E. J. Esienbraum, Oklahoma State University, USA, was recrystallized from toluene.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Thioxanthene; $C_{13}H_{10}S$; [261-31-4]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.6	0.9324	0.0676	339.8	0.8013	0.1987
311.9	0.9178	0.0822	350.4	0.7228	0.2772
322.7	0.8837	0.1163			
330.0	0.8524	0.1476			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Thioxanthene; $C_{13}H_{10}S$; [261-31-4]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.2	0.9073	0.0927	338.4	0.7860	0.2140
317.4	0.8829	0.1171	342.3	0.7593	0.2407
325.3	0.8567	0.1433			
332.1	0.8208	0.1792			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

TRIPHENYLENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

benzene
benz[a]anthracene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

59322 59-430

COMPONENTS:

(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
20.0	0.0056

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
312.6	0.9860	0.0140	356.0	0.9503	0.0497
320.8	0.9819	0.0181			
337.0	0.9711	0.0289			
342.6	0.9659	0.0341			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visunoting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Rutgerswerke A.G., Germany, was passed over an alumina column with benzene as eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (2) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]	Sturrock, M.G.; Lawe, T. *Can. J. Res., Sect. B.* 1939, *17*, 71-74.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
433.2	433.2	1.000	0.000
427.2	421.2	0.900	0.100
423.2	404.2	0.850	0.150
419.2	403.2	0.800	0.200
414.2	403.2	0.750	0.250
405.2	403.2	0.650	0.350
404.2	403.2	0.630	0.370
427.2	403.2	0.500	0.500
454.2	403.2	0.300	0.700
456.2	412.2	0.275	0.725
457.2	425.2	0.250	0.750
470.2	470.2	0.000	1.000

[a] Binary system shows incomplete solid solution from *circa* x_1 = 0.00 to x_1 = 0.15, and from x_1 = 0.71 to x_1 = 1.00. T_{in} refers to the temperature which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Melting points and freezing points were obtained by determining temperatures of incipient fusion and complete liquefaction using capillary tube method. Temperature very slowly raised and material observed through a low power microscope.	(1) Obtained from heavy crude oil, and was recrystallized from alcohol before use. (2) Obtained from heavy crude oil, and was fractionally recrystallized from alcohol before use.
	ESTIMATED ERRORS:
	T/K: precision ± 0.5 (Compiler). x_1: ± 0.005 (Compiler).

XANTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
1,2,3,4-tetrahydronaphthalene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Xanthene; $C_{13}H_{10}O$; [92-83-1]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
331.7	0.7951	0.2049	354.3	0.3826	0.6174
339.0	0.6936	0.3064	359.7	0.2784	0.7216
344.9	0.5897	0.4103			
350.3	0.4867	0.5133			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Xanthene; $C_{13}H_{10}O$; [92-83-1]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
316.6	0.8648	0.1352	346.7	0.5365	0.4635
322.3	0.8218	0.1782	351.5	0.4387	0.5613
332.4	0.7258	0.2742			
339.7	0.6188	0.3812			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Xanthene; $C_{13}H_{10}O$; [92-83-1]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
299.6	0.8342	0.1658	336.0	0.5621	0.4379
315.2	0.7471	0.2529	349.6	0.3876	0.6124
315.9	0.7466	0.2534			
324.9	0.6695	0.3305			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Xanthene; $C_{13}H_{10}O$; [92-83-1]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
304.6	0.7798	0.2202	348.9	0.3953	0.6047
318.3	0.7124	0.2876	349.9	0.3714	0.6286
331.8	0.5978	0.4022			
340.9	0.4986	0.5014			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Xanthene; $C_{13}H_{10}O$; [92-83-1]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
312.1	0.7619	0.2381	345.3	0.4420	0.5580
315.3	0.7437	0.2563	355.6	0.3075	0.6925
332.2	0.6090	0.3910			
340.2	0.5191	0.4809			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Xanthene; $C_{13}H_{10}O$; [92-83-1]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
301.1	0.8082	0.1918	347.5	0.4069	0.5931
318.2	0.7031	0.2969	355.6	0.2997	0.7003
329.7	0.6073	0.3927			
339.8	0.5091	0.4909			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

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T/K: precision ± 0.1.
x_1: ± 0.0003.

SYSTEM INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

REGISTRY NUMBER INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

AUTHOR INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

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