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SOLUBILITY DATA SERIES

Volume 59

POLYCYCLIC AROMATIC HYDROCARBONS: BINARY NON-AQUEOUS SYSTEMS PART II: SOLUTES F-Z

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CONTENTS

	Introduction to the Solubility of Solids in Liquids	viii
	Preface	xv
	Basic Thermodynamic Principles	xvii
	Melting Temperatures and Entropies of Fusion	xviii
	Solubilities in Single Solvents	xxi
	Scatchard-Hildebrand Solubility Parameter Model	xxii
	Solubilities in Binary Solvent Mixtures	xxiii
	Mathematical Representation of Solubility Data in Binary Solvents	xxvi
	References	xxix
1	Fluoranthene Solubilities in Pure and Binary Solvent Mixtures	1
	Saturated Hydrocarbons (including Cycloalkanes)	3
	Aromatic Hydrocarbons	3
	Ethers	15
	Haloalkanes and Haloaromatic Hydrocarbons	15
	Alcohols	16
	Ketones	19
	Miscellaneous Pure Solvents	19
2	Fluorene Solubilities in Pure and Binary Solvent Mixtures	32
	Saturated Hydrocarbons (including Cycloalkanes)	34
	Aromatic Hydrocarbons	35
	Haloalkanes and Haloaromatic Hydrocarbons	50
	Alcohols	51
	Miscellaneous Pure Solvents	52
3	Indole Solubilites in Pure and Binary Solvent Mixtures	65
	Aromatic Hydrocarbons	66
	Ethers	73
	Alcohols	74
	Micellaneous Pure Solvents	74
4	Naphthacene Solubilities in Pure and Binary Solvent Mixtures	77
	Saturated Hydrocarbons (including Cycloalkanes)	78
	Aromatic Hydrocarbons	78
	Alcohols	79
5	Naphthalene Solubilities in Pure and Binary Solvent Mixtures	80
	Saturated Hydrocarbons (including Cycloalkanes)	83
	Aromatic Hydrocarbons	97
	Esters	123
	Ethers	126
	Haloalkanes and Haloaromatic Hydrocarbons	129
	Alcohols	143
	Ketones	167
	Miscellaneous Pure Solvents	168
	Binary Solvents	193

6	Perylene Solubilities in Pure and Binary Solvent Mixtures	203
	Saturated Hydrocarbons (including Cycloalkanes)	204
	Aromatic Hydrocarbons	204
	Alcohols	205
7	Phenanthrene Solubilities in Pure and Binary Solvent Mixtures	206
	Saturated Hydrocarbons (including Cycloalkanes)	208
	Aromatic Hydrocarbons	213
	Haloalkanes and Haloaromatic Hydrocarbons	219
	Alcohols	221
	Miscellaneous Pure Solvents	222
8	1,10-Phenanthroline Solubilities in Pure and Binary Solvent Mixtures	241
	Binary Solvent Mixtures	242
9	Phenothiazine Solubilities in Pure and Binary Solvent Mixtures	245
	Miscellaneous Pure Solvents	246
10	Phenoxanthiin Solubilities in Pure and Binary Solvent Mixtures	250
	Miscellaneous Pure Solvents	251
11	Phenoxazine Solubilities in Pure and Binary Solvent Mixtures	254
	Miscellaneous Pure Solvents	255
12	Pyrene Solubilities in Pure and Binary Solvent Mixtures	258
	Saturated Hydrocarbons (including Cycloalkanes)	260
	Aromatic Hydrocarbons	266
	Esters	271
	Ethers	273
	Haloalkanes and Haloaromatic Hydrocarbons	274
	Alcohols	277
	Ketones	285
	Miscellaneous Pure Solvents	286
	Binary Solvent Mixtures	300
13	Thianthrene Solubilities in Pure and Binary Solvent Mixtures	312
	Saturated Hydrocarbons (including Cycloalkanes)	313
	Aromatic Hydrocarbons	317
	Miscellaneous Pure Solvents	318
14	Thioxanthene Solubilities in Pure and Binary Solvent Mixtures	320
	Saturated Hydrocarbons (including Cycloalkanes)	321
	Aromatic Hydrocarbons	322
	Miscellaneous Pure Solvents	323
15	Triphenylene Solubilities in Pure and Binary Solvent Mixtures	324
	Saturated Hydrocarbons (including Cycloalkanes)	325
	Aromatic Hydrocarbons	325
16	Xanthene Solubilities in Pure and Binary Solvent Mixtures	327
	Saturated Hydrocarbons (including Cycloalkanes)	328
	Aromatic Hydrocarbons	329
	Miscellaneous Pure Solvents	330

System Index	331
Registry Number Index	338
Author Index	342
Solubility Data Series: Published and Forthcoming Volume	s 346

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: That of the end of the known elements, in order of atomic number.

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

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

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

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

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

Errors in calculations, fitting equations, etc. are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler" or by the compiler's name in parentheses or in a footnote. In addition, compiler-calculated values of mole or mass fractions are included if the original data do not use these units. If densities are reported in the original paper,

conversions from concentrations to mole fractions are included, but otherwise this is done in the evaluation, with the values and sources of the densities being quoted and referenced.

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

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

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

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

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

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

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

Evaluations

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

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

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

Critical Evaluation:

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

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

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

- (b) Fitting equations. If the use of a smoothing equation is justifiable the evaluator may provide an equation representing the solubility as a function of the variables reported on all the compilation sheets, stating the limits within which it should be used.
 - (c) Graphical summary. In addition to (b) above, graphical summaries are often given.
 - (d) Recommended values. Data are recommended if the results of at least two independent

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

- (e) References. All pertinent references are given here, including all those publications appearing in the accompanying compilation sheets and those which, by virtue of their poor precision, have been rejected and not compiled.
- (f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units (3) when the data can be accurately converted.

QUANTITIES AND UNITS USED IN COMPILATION AND EVALUATION OF SOLUBILITY DATA

Mixtures, Solutions and Solubilities

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

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

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

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

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

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

Physicochemical Quantities and Units

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

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

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

$$x_1 = n_1 / \sum_{s=1}^{c} n_s \tag{1}$$

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_{1+} cations and ν_{1-} anions, with $\nu_{1} = \nu_{1+} + \nu_{1-}$ and a mixture of p non-electrolytes k, of which some may be considered as solvent components, a generalization of the definition in (7) gives:

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

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

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

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

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

$$x_1 = \frac{v_{+2}x_{o1}}{v_{+2} - (v_2 - 1)x_{+2}} \qquad x_2 = \frac{x_{+2}}{v_{+2} - (v_2 - 1)x_{+2}}$$
 [5]

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

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

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

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

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

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

$$x_{v,1} = x_1 / \sum_{s=1}^{p} x_s$$
 [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), $m_1^{(3)}$:

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

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

$$\overline{M} = x_{v2}M_2 + (1 - x_{v2})M_3$$
 [11]

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

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

$$c_1 = [formula of solute] = n_1/V$$
 [12]

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

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

$$\rho_1 = g_1/V = c_1 M_1/V \tag{13}$$

SI base units: kg m⁻³.

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

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

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

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

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

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

$$I_{m} = |z_{2}z_{1}| vm_{i}, I_{c} = |z_{2}z_{1}| vc_{i}$$
 [16]

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

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

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

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

12. Density, ρ :

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

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

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

Thermodynamics of Solubility

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

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

		x_i	w _i	m_i	c_i
	$x_i =$	x_i	$\frac{1}{1 + \frac{M_i}{M_c} \left(\frac{1}{w_i} - 1 + \sum_{j \neq i}^{c-1} \left(\frac{M_c}{M_j} - 1\right) \frac{w_j}{w_i}\right)}$	$\frac{1}{1 + \frac{1}{m_i M_c} + \sum_{j \neq i}^{c-1} \frac{m_j}{m_i}}$	$\frac{1}{1 + \frac{1}{M_c} \left(\frac{\rho}{c_i} - M_i\right) + \sum_{j \neq i}^{c-1} \frac{c_j}{c_i} \left(1 - \frac{M_j}{M_c}\right)}$
×	$w_i = $	$\frac{1}{1 + \frac{M_c}{M_i} \left(\frac{1}{x_i} - 1 + \sum_{j \neq i}^{c-1} \left(\frac{M_j}{M_c} - 1 \right) \frac{x_j}{x_i} \right)}$	w_i	$\frac{1}{1 + \frac{1}{m_i M_i} \left(1 + \sum_{j \neq i}^{c-1} m_j M_j\right)}$	$\frac{c_i M_i}{\rho}$
xiv	$m_i =$	$\frac{1}{M_c \left(\frac{1}{x_i} - 1 - \sum_{j \neq i}^{c-1} \frac{x_j}{x_i}\right)}$	$\frac{1}{M_i \left(\frac{1}{w_i} - 1 - \sum_{j \neq i}^{c-1} \frac{w_j}{w_i}\right)}$	$m_{\tilde{i}}$	$\frac{1}{\frac{1}{c_i} \left(\rho - \sum_{j \neq i}^{c-1} c_j M_j \right) - M_i}$
	c _i =	$\frac{\rho}{M_i + M_c \left(\frac{1}{x_i} - 1 + \sum_{j \neq i}^{c-1} \left(\frac{M_j}{M_c} - 1\right) \frac{x_j}{x_i}\right)}$	$\frac{\rho w_i}{M_i}$	$\frac{\rho}{\frac{1}{m_i} \left(1 + \sum_{j \neq i}^{c-1} M_j m_j\right) + M_i}$	$c_{m{i}}$

 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

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

(3) m le fraction

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

or (4) volume fraction

$$\phi_1 = n_1 V_1 / (n_1 V_1 + n_2 V_2 + n_3 V_3 + \dots)$$
 [3]

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

$$\phi_1 = n_1 V_{m,1} / (n_1 V_{m,1} + n_2 V_{m,2} + n_3 V_{m,3} + \dots)$$
 [4]

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

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

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

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

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

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

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

The thermodynamic criterion for solubility equilibrium of a component 1 in any system at temperature T, standard pressure p^{o} is:

$$\mu_1^*(\text{solid}, T, p^0) = \mu_1(\text{sln}, T, p^0)$$
 [6]

We choose the standard state for component 1 as the chemical potential of supercooled liquid 1 and T, p^0 . Thus

$$\mu_1^*(s,T,p^0) = \mu_1^0(1,T,p^0) + RT \ln a_1$$
 [7]

from which the standard Gibbs energy of fusion is

$$\Delta_{fus}G_{m}^{o}/RT = -\ln a_{1}$$
 [8]

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

$$\ln a_1(s) = \ln (\gamma_1 x_1) = -\Delta_{fus} H_m^o (T_m - T) / R T T_m + \Delta C_p (T_m - T) / R T$$

$$- (\Delta C_p / R) \ln (T_m / T)$$
[9]

for the solubility of a crystalline solute in a liquid solvent, where $\Delta_{fus}H_m^o$ is the standard enthalpy of fusion. In the above expression γ_1 is the activity coefficient of the solute. The expression for $a_1(s)$ 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 $\Delta_{\rm fus}H_{\rm m}^{\rm o}$ 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	$\Delta_{\text{fus}} H_{\text{m}}^{\text{o}}/\text{kJ mol}^{-1}$	$\Delta_{\text{fus}} s_{\text{m}}^{\text{o}} / \text{J mol}^{-1} \text{ K}^{-1}$
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

^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:

$$\Delta_{\text{fus}} S_{\text{m}}^{\ 0} = -R \ln P_{\text{fus}}$$
 [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

$$\Delta_{\text{fus}} S_{\text{m}}^{\, \circ} = \Delta_{\text{trans}} S_{\text{m}}^{\, \circ} + \Delta_{\text{rot}} S_{\text{m}}^{\, \circ} \tag{11}$$

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 $\Delta_{\text{trans}} S_m^o = 14.6 \text{ J mol}^{-1} \text{ K}^{-1}$ 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 \pm 10° variation in ϕ and θ corresponds to a spherical segment that is roughly 0.00754 times that of a sphere of the same radius, or roughly a rotational entropy of fusion of $\Lambda_{fix}S_{ix}^{0} = 41.8 \text{ J mol}^{-1}$

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

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

For acyclic and aromatic hydrocarbons

$$\Delta_{\text{fus}} S_{\text{m}}^{\text{o}} = \Sigma \ n_{i} \ C_{i} \ G_{i} + \Sigma \ n_{j} \ C_{j} \ G_{j} + \Sigma \ n_{k} \ C_{K} \ G_{k}$$
 [12] For cyclic hydrocarbons

 $\Delta_{\text{fus}} S_{\text{m}}^{\text{o}} = [8.41 + 1.025 (n - 3)] + \sum_{i} n_{i} C_{i} G_{i} + \sum_{i} n_{j} C_{j} G_{j} + \sum_{i} n_{k} C_{k} G_{k}$ [13] For polycyclic molecules

$$\Delta_{\text{fus}} S_{\text{m}}^{\text{o}} = [8.41 \text{ N} + 1.025 (R - 3N)] + \sum_{i} C_{i} G_{i} + \sum_{i} C_{j} G_{j} + \sum_{i} C_{k} G_{k}$$

where $K = \sum_{i} n_{k}$, 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 $\Delta_{fus}S_m^0$ 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 $\Delta_{fus}S_m^0$ and $\Delta_{fus}H_m^0$. 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 (γ_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

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

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

provides a more realistic description of solution ideality in polymer solutions. The corresponding expression for solubility (as a volume fraction eqn. [3]) is given by $\ln \phi_1 + (1-\phi_1)(1-V_{m,1}/V_{m,2}) = -\Delta_{fus}H_m^o (T_m-T)/RT T_m + \Delta C_p (T_m-T)/RT$

[17]

Chiou and Manes (15) compared experimental solubilities of 11 crystalline nonpolar polycyclic aromatic compounds and their derivatives in glycerol trioleate ($V_{m,s}$ = 966 cm³ mol⁻¹) to predictions based upon eqns. [9] and [17]. The authors' calculations revealed that the observed mole fraction solubilities are considerably higher than the predictions of eqn. [9] (with ΔC_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 ΔC_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

- $(\Delta C_{\rm p}/R)$ ln $(T_{\rm m}/T)$

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 net alous, and there have been numerous disagreements in the published literature regarding the separation of specific and nonspecific interactions.

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

RT ln $(a_1(s)/x_1) = V_{m,1} (1 - \phi_1)^2 (\delta_1 - \delta_{solvent})^2$ [18] where $\delta_{solvent}$ and δ_1 refer to the solubility parameters of the solvent and supercooled liquid solute, respectively, $V_{m,1}$ is the molar volume of the supercooled liquid solute, x_1 is the saturation mole fraction solubility, and ϕ_1 is the solute's volume fraction solubility calculated using the ideal molar volume approximation (eqn. [4]). For solvent components, the liquid molar volumes and solubility parameters are often tabulated in the literature (for example, see both Hoy (18) and Barton (17)), and when not available, they can be calculated directly from density and vapor pressure measurements on the pure liquid. Molar volumes of supercooled liquid solutes, $V_{m,1}$, on the other hand, are estimated either by group contribution methods or by the experimentally determined apparent 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 cm³ mol⁻¹ and $V_{m,naphthalene}$ = 123.0 cm³ 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 $\delta_{\rm solvent}$:

 $\delta_{\rm solvent} = (\phi_2 \ \delta_2 + \phi_3 \ \delta_3)/(\phi_2 + \phi_3) = \phi_2^{(s)} \ \delta_2 + \phi_3^{(s)} \ \delta_3$ [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	$V_{m,2}/cm^3 \text{ mol}^{-1}$	x ₁ (exp) ^b	x ₁ (calc)
oichloromethane	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
richloromethane	18.74	80.64	0.339	0.305
ethylbenzene	18.27	106.84	0.292	0.295
thylbenzene	18.08	123.08	0.289	0.289
etrachloromethane	17.49	97.08	0.255	0.275
yclohexane	16.75	108.76	0.147	0.242
ethylcyclohexane	15.95	128.32	0.147	0.189
-Octane	15.42	163.48	0.142	0.146
-Heptane	15.34	147.48	0.130	0.144
-Hexane	14.87	131.51	0.122	0.119
arbon disulfide	20.29	60.62	0.283	0.311

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

TABLE III. Comparison Between Experimental and Predicted Biphenyl Solubilities

Solvent	δ ₂ a	$V_{m,2}/cm^3 \text{ mol}^{-1}$	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	

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

b Experimental solubilites were determined by Chang (26).

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]

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

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

$$- \phi_2^{(s)} \phi_3^{(s)} (\delta_2 - \delta_3)^2]$$
 [21]

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

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

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

$$G_{23}^{E} = (x_{2}^{(s)} V_{m,2} + x_{3}^{(s)} V_{m,3}) \phi_{2}^{(s)} \phi_{3}^{(s)} (\delta_{2} - \delta_{3})^{2}$$
 [23] in terms of solubility parameters.

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

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

$$-\ln x_1 = -\ln a_1(s) + (V_{m,1} \phi_{solvent}^2/RT) \left[\delta_{solvent}^2 + \delta_1^2 - 2 \sum A_i \delta_{solvent}^1\right]$$
 [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 A₁-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

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

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

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

$$\ln x_1 = x_2^{(8)} \ln (x_1)_2 + x_3^{(8)} \ln (x_1)_3 + x_2^{(8)} x_3^{(8)} \Sigma S_i (x_2^{(8)} - x_3^{(8)})^{\frac{1}{2}}$$
 [28]

or Modified Wilson equation

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

where the various S_i and Λ_{ij}^{adj} "curve-fit" parameters can be evaluated via least squares analysis. A summarized comparison presenting the descriptive abilities of eqns. [29] and [28] is summarized in Tables IV and V, respectively. For pyrene, a value of $a_i(s)$ = 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	1.4
	1.348	
n-Heptane + 1-propanol	1.249	0.7
	1.577	
n-Octane + 1-propanol	1.032	1.1
	1.936	
Cyclohexane + 1-propanol	1.749	0.6
	1.281	
Methylcyclohexane + 1-propanol	1.605	0.4
	1.450	
2,2,4-Trimethylpentane + 1-propanol	0.804	0.6
	1.744	
n-Hexane + 2-propanol	1.080	0.4
	1.628	
n-Heptane + 2-propanol	1.072	0.9
	1.908	
n-Octane + 2-propanol	0.936	1.1
	2.248	
Cyclohexane + 2-propanol	1.464	0.8
	1.556	
Methylcyclohexane + 2-propanol	1.404	1.0
	1.744	
2,2,4-Trimethylpentane + 2-propanol	0.904	0.8
	1.752	

a Adjustable parameters for the Modified Wilson equation are ordered as $\Lambda_{23}^{\text{adj}}$ and then $\Lambda_{32}^{\text{adj}}$. See eqn. [29] in text. b % Dev. = $(100/\text{N}) \Sigma \mid \ln [x_{\text{A}}(\text{cal})/x_{\text{A}}(\text{exp})] \mid$.

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

^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) Σ | ln [x_A (cal)/ x_A (exp)] |.

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

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. <u>Ketones</u>
 - . 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:			ORIGINAL MEASUREMENTS: McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 3854-3857.			
(1) Fluorant	hene; C ₁₆ H ₁₀ ;	[206-44-0]				
(2) Cyclohex	ane; C ₆ H ₁₂ ; [3	10-82-7]				
VARIABLES:			PREPARED I	BY:		
Temperature			W.E. Acree, Jr.			
EIPERIMENTAL '	VALUES					
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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				
		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:

- 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 \pm 0.1. x_1 : \pm 0.0003 (compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Fluoranthene; C ₁₆ F	i ₁₀ ; [206-44-0]	McLaughlin, E.; Zainal, H.A.		
(2) Benzene; C ₆ H ₆ ; [7]	-43-2]	J. Chem. Soc. <u>1959</u> , 863-867.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		-		
T/K	x ₂	<i>x</i> 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:

- 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 \pm 0.1. x_1 : \pm 0.0003 (compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:						
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Benzene; C ₆ H ₆ ; [71-43-2] VARIABLES: Temperature		Kravchenko, V.M.; Pastukhova, I.S. J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) PREPARED BY: 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

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:

- 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 \pm 0.2 (Compiler). x₁: \pm 0.002 (Compiler).

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3] VARIABLES:		ORIGINAL MEASUREMENTS: Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259. PREPARED BY:					
				T/K = 293		W.E. Acree, Jr.	
					JES		
				EIPERIMENT AL VALU			
EIPERIMENT AL VALU t/° C	x ₂	<i>x</i> 1					

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. after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS: ORIGINAL MEASUREMENTS: Kravchenko, V.M.; Pastukhova, I.S. (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2] J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₁ x₂ 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) 0.650 0.350 332.7 (2) 332.2 0.618 0.382 Eutectic 334.5 0.601 0.399 (1) 0.552 340.4 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:

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

ESTIMATED ERRORS:

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

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Naphthalene; C ₁₀ H ₈ ; [91-20-3] VARIABLES: Temperature		ORIGINAL MEASUREMENTS: Kravchenko, V.M.; Pastukhova, I.S. J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) PREPARED BY:						
					W.E. Acree, Jr.			
					EXPERIMENTAL VALUES			
					T/K	<i>x</i> ₂	<i>x</i> 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

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:

- 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:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] Kravchenko, V.M.; Pastukhova, I.S. (2) 2-Methylnaphthalene; C₁₁H₁₀; [91-57-6] J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K *x*₁ x_2 0.000 307.3 1.000 (2) 0.899 298.4 0.101 (2) 296.5 0.871 0.129 (2) 293.8 0.835 0.165 (2) 0.799 Eutectic 292.5 0.201 297.9 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) 0.242 0.758 365.1 (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

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:

- 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:

COMPONENTS ORIGINAL MEASUREMENTS: Kravchenko, V.M.; Pastukhova, I.S. (1) Fluoranthene; C16H10; [206-44-0] (2) 2,7-Dimethylnaphthalene; C₁₂H₁₂; J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. [582-16-1] (English translation) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x_2 x₁ 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)

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

0.328

0.242

0.136

0.000

0.672

0.758

0.864

1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

356.4

363.8

372.6

383.2

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:

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

(1)

(1)

(1)

(1)

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

ESTIMATED ERRORS:

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] VARIABLES: Temperature		ORIGINAL MEASUREMENTS:					
		Kravchenko, V.M.; Pastukhova, I.S. J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) PREPARED BY: W.E. Acree, Jr.					
				EXPERIMENTAL VALUES			
				T/K	x ₂	<i>x</i> 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

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.

METHOD: APPARATUS/PROCEDURE

SOURCE AND PURITY OF MATERIALS:

- 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:

ORIGINAL MEASUREMENTS: COMPONENTS: Kravchenko, V.M.; Pastukhova, I.S. (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Anthracene; C₁₄H₁₀; [120-12-7] J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₂ x₁ 489.7 1.000 0.000 (2) 475.1 0.822 0.178 (2) 467.4 0.731 0.269 (2) 459.7 0.355 (2) 0.645 0.544 449.4 0.456 (2) 435.2 0.434 (2) 0.566 (2) 419.9 0.329 0.671 395.7 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)

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

1,000

0.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

383.2

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:

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

(1)

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

ESTIMATED ERRORS:

 x_1 : \pm 0.002 (Compiler).

14						
COMPONENTS:		ORIGINAL MEA	SUREMENTS:			
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] VARIABLES: Temperature		Kravchenko, V.M.; Pastukhova, I.S. J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) PREPARED BY:				
					W.E. Acree,	Jr.
					EXPERIMENTAL VALUES	
		T/K	x ₂	<i>x</i> 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.* 1939, 13, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

- 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:

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] VARIABLES: Temperature		ORIGINAL ME	ASUREMENTS:			
		Kravchenko, V.M.; Pastukhova, I.S. J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) PREPARED BY:				
					W.E. Acree, Jr.	
					EIPERIMENTAL VALUES	
		T/K	x ₂	<i>x</i> 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:

- 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:

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] VARIABLES: Temperature		ORIGINAL MEASUREMENTS:					
		Kravchenko, V.M.; Pastukhova, I.S. Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669. (English translation) PREPARED BY: W.E. Acree, Jr.					
				EXPERIMENTAL VALUES			
				T/K	*2	<i>x</i> 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)				

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:

- 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:

COMPONENTS:

- (1) Fluoranthene; C₁₆H₁₀; [206-44-0]
- (2) 1,4-Dioxane; C₂H₈O₂; [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

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

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:

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: \pm 1. c₁: \pm 5% (relative error; compiler).

COMPONENTS:

- (1) Fluoranthene; C₁₆H₁₀; [206-44-0]
- (2) Tetrachloromethane; CCl₄;
 [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	× ₂	<i>×</i> 1
305.0	0.8968	0.1032
313.4	0.8576	0.1424
320.2	0.8179	0.1821
326.2	0.7722	0.2278

T/K 333.6

x₂ 0.7016

0.2984

 x_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:

- 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 \pm 0.1. x_1 : \pm 0.0003 (compiler).

16 COMPONENTS: ORIGINAL MEASUREMENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Chlorobenzene; C₆H₅Cl; [108-90-7] Environ. Sci. Technol. 1990, 24, 639-646. VARIABLES: PREPARED BY: T/K = 296W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(mol dm^{-3})$ t/°C 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:

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: \pm 1. c₁: \pm 5% (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Methanol; CH₄O; [67-56-1] 	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.

t/°C c₁/(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:

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: \pm 1. c₁: \pm 5% (relative error; compiler).

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Ethanol; C ₂ H ₆ O; [64-17-5] VARIABLES: T/K = 293		ORIGINAL MEASUREMENTS:				
		Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259. PREPARED BY: W.E. Acree, Jr.				
				EXPERIMENTAL VALUES		
				t/° C	x ₂	x ₁
				20.0	0.9949	0.00514

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 \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Fluoranthene; C₁₆H₁₀; [206-44-0] 1-Octanol; C₈H₁₈O; [111-87-5] 	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. 1985, 19, 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
4.100	- //

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:

- 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: \pm 0.1 (compiler). c_1 : \pm 3 % (relative error; compiler).

18		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) 1-Octanol; C ₈ H 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	(mol dm ⁻³)	
23.0 0.198		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.	
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a 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	(2) Purity and chemical source not given, purification procedure not specified.	
fluorescence or uv detection.	ESTIMATED ERRORS:	

AUXILIARY INFORMATION			
23.0	0.0534		
t/°C	$c_1/(\text{mol dm}^{-3})$		
EXPERIMENTAL VALUES			
T/K = 296	W.E. Acree, Jr.		
VARIABLES:	PREPARED BY:		
 (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) 1-Hydroxy-2-methylbenzene; C₇H₈O; [95-48-7] 	P.V.; Yalkowsky, S.H. Environ. Sci. Technol. 1990, 24, 639-646.		
COMPONENTS:	ORIGINAL MEASUREMENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline,		

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 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 my detection. fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

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

- Purity not given, commercial sample of unspecified source, was used as
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

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

	19	
COMPONENTS:	ORIGINAL MEASUREMENTS: Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259. PREPARED BY: W.E. Acree, Jr.	
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]		
(2) 2-Propanone; C ₃ H ₆ O; [67-64-1]		
VARIABLES:		
T/K = 293		
EXPERIMENTAL VALUES	-	
t/° C x ₂	<i>x</i> ₁	
20.0 0.9289	0.0711	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	(1) 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.	
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K : precision \pm 0.05. x_1 : \pm 3 % (relative error; compiler).	

(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Pyridine; C ₅ H ₅ N; [110-86-1] VARIABLES:		ORIGINAL MEASUREMENTS:							
		Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259. PREPARED BY:							
					T/K = 293		W.E. Acree, Jr.		
					EXPERIMENTAL VALUES		· · ·		
t/° C	x ₂	x ₁							
20.0	0.842	0.158							
	AUXIL	IARY INFORMATION							
//									

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 \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

20			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]	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.		
EIPERIMENTAL VALUES			
t/°C	(mol dm ⁻³)		
23.0 1.9	8		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a 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 reversedphase liquid chromatography with either	(2) Purity and chemical source not given, purification procedure not specified.		
fluorescence or uv detection.	ESTIMATED ERRORS:		
	T/K: ± 1. c ₁ : ± 5% (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Dimethyl sulfoxide; C ₂ H ₆ OS; [67-68-5]	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.		
EIPERIMENTAL VALUES	,		
t/°C c ₁ /((mol dm ⁻³)		
23.0 1.09	9		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a 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	(2) Purity and chemical source not given, purification procedure not specified.		
fluorescence or uv detection.	ESTIMATED ERRORS:		
	T/K: ± 1. c ₁ : ± 5% (relative error; compiler).		

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] Shinomiya, C. (2) 1,3-Dinitrobenzene; C₆H₄N₂O₄; [99-65-0] J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase x₁ x₂ 0.000 363.2 1.000 (2) 0.121 356.2 0.879 (2) 0.784 0.216 350.2 (2) 0.752 0.248 346.2 (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 0.478 0.522 1:1 Compound 350.2 0.502 0.498 1;1 Compound 0.430 0.570 349.2 (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.

0.615

0.693

1.000

(2)

(2)

(2)

0.385

0.307

0.000

349.2

352.7

382.7

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE 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). x₁: ± 0.002 (Compiler).

22 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] Shinomiya, C. (2) 1,4-Dinitrobenzene; C₆H₄N₂O₄; [100-25-4] J. Chem. Soc. Japan 1940, 15, 259-270. VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES Solid Phase T/K x₁ x₂ 446.7 1.000 0.000 (2) 426.2 0.706 0.294 (2) 0.432 411.2 0.568 (2) 0.406 0.594 388.2 (2) 370.2 0.323 0.667 (2) 0.231 0.769 363.2 (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 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

			Ζ.		
COMPONENTS:		ORIGINAL ME	Easurements:		
(1) Fluoranthene; C ₁₆ F	(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	Shinomiya, C.			
(2) 1,3,5-Trinitroben [99-35-4]	2) 1,3,5-Trinitrobenzene; C ₆ H ₃ N ₃ O ₆ ; [99-35-4]		J. Chem. Soc. Japan <u>1940</u> , 15, 259-270.		
VARIABLES:		PREPARED B	Yı		
Temperature		W.E. Acres	e, Jr.		
EXPERIMENTAL VALUES					
T/K	x ₂	<i>×</i> 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.

METHOD: APPARATUS/PROCEDURE 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). x₁: ± 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] Shinomiya, C. (2) 1,2,3,5-Tetranitrobenzene; C₆H₂N₄O₈; [3698-53-1] J. Chem. Soc. Japan 1940, 15, 259-270. VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K Solid Phase ×₂ ×₁ 0.000 399.2 1.000 (2) 385.2 0.939 0.061 (2) 389.2 0.836 0.164 (2) 1:1 Compound 393.2 0.680 0.320 393.2 0.328 1:1 Compound 0.672 1:1 Compound 405.2 0.561 0.439 405.2 0.522 0.478 1:1 Compound 407.2 0.501 0.499 1:1 Compound 1:1 Compound 403.2 0.402 0.598 397.2 0.360 0.640 1:1 Compound 383.2 0.284 0.716 1:1 Compound 0.217 1:1 Compound 370.2 0.783 361.2 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	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; C₁₆H₁₀; [206-44-0] (2) 2,4-Dinitromethylbenzene; J. Chem. Soc. Japan 1940, 15, 259-270. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr.

EIPERIM	ENTAL VALUES		•		
	T/K	* 2	× 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)	
ľ	363.2	0.198	0.802	(1)	
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 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). x₁: ± 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] Shinomiya, C. (2) 2,4-Dinitrophenol; C₆H₄N₂O₅; [51-28-5] J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES Solid Phase T/K x_2 x₁ 0.000 1.000 386.7 (2) 0.126 379.2 0.874 (2) 375.0 0.790 0.210 (2) 367.2 0.695 0.305 (2) 1:1 Compound 360.2 0.622 0.378 0.400 1:1 Compound 360.7 0.600 0.495 1:1 Compound 364.2 0.505 0.491 1:1 Compound 365.2 0.509 361.2 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.

METEOD: APPARATUS/PROCEDURE 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). x₁: ± 0.002 (Compiler).

				2
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]		ORIGINAL MEASUREMENTS: Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270.		
VARIABLES:				
Temperature		W.E. Acree	e, Jr.	
EXPERIMENTAL VALUES				
T/K	<i>x</i> ₂	<i>x</i> 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)	
i				

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.

METHOD: APPARATUS/PROCEDURE 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). x₁: ± 0.002 (Compiler).

COMPONENTS: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) 2,4,6-Trinitromethoxybenzene; C ₇ H ₅ N ₃ O ₇ ; [606-35-9] VARIABLES: Temperature		ORIGINAL MEASUREMENTS: Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: W.E. Acree, Jr.	
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)
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. (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). x₁: ± 0.002 (Compiler).

(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) 2,4,6-Trinitroaniline; C ₆ H ₄ N ₄ O ₆ ; [489-98-5]		ORIGINAL ME	ORIGINAL MEASUREMENTS:		
		Shinomiya, C.			
		J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY:			
				Temperature	
EXPERIMENTAL VALUES		,			
T/K	x ₂	<i>x</i> 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		

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.

0.738

0.842

0.901

0.947

1.000

1:1 Compound

1:1 Compound

1:1 Compound

(1)

(1)

441.2

414.2

390.7

378.2

382.7

0.262

0.158

0.099

0.053

0.000

AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE 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). x₁: ± 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: Shinomiya, C. (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) 2-Chloro-1,3,5-trinitrobenzene; C₆H₂ClN₃O₆; [88-88-0] J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₂ x₁ 1.000 0.000 356.2 (2) 0.173 1:1 Compound 0.827 346.7 370.2 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 0.536 1:1 Compound 392.2 0.464 1:1 Compound 392.2 0.460 0.540 0.375 0.625 1:1 Compound 385.2 379.2 0.330 0.670 1:1 Compound 371.2 0.846 0.154 (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	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.	
	ESTINATED ERRORS:	
	x/K : precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).	

(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) 3-Methyl-2,4,6-trinitrophenol; C ₇ H ₅ N ₃ O ₇ ; [602-99-3]		ORIGINAL MEASUREMENTS: Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270.						
					VARIABLES:		PREPARED BY	(1
					Temperature		W.E. Acree	e, Jr.
EXPERIMENTAL VALUES								
T/K	* 2	<i>×</i> 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			
METBOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
No experimental details given in paper.	 Purity and chemical source were not specified in paper. 		
	(2) Purity and chemical source were not specified in paper.		
	ESTIMATED ERRORS:		
	T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).		

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

tetrachloromethane chlorobenzene

G. Alcohols

methanol ethanol 1-octanol

- H. <u>Ketones</u>
- 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:			ORIGINAL MEASUREMENTS:			
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7] VARIABLES:			Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.			
			PREPARED B	Y:		
Temperature			W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES					
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	ı		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			(1) 97.9 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and recrystal- lized from toluene. (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.			
noting the te	were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.			ERRORS: dision ± 0.1.		

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ H ₁₀ ;	[86-73-7]	McLaughlin, E.; Zainal, H.A.
(2) Cyclohexane; C ₆ H ₁	2; [110-82-7]	J. Chem. Soc. <u>1960</u> , 3854-3857.
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		<u> </u>
T/K	* ₂	<i>x</i> 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
ŒTHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:
	centrations sealed	(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.
noting the temperatur trace of solid solute	e at which the last	ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 0.0003 (compiler).

₀ ; [86-73-7]	Coon	, J.E.; Auwaerter,	JE · McLaughlin E	
		, 0.2.,	U.D., McDaughiin, D.	
(2) Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8]		Fluid Phase Equilibr. 1989,		
	PREPA	RED BY:		
	W.E.	Acree, Jr.		
<i>x</i> ₁	T/K	x ₂	<i>x</i> ₁	
9157 0.084	353.	0 0.5555	0.4445	
8509 0.149	366.	2 0.3329	0.6671	
7756 0.224	4			
6856 0.314	4			
	*1 9157 0.084 8509 0.149 7756 0.224	PREPA W.E. *1	PREPARED BY: W.E. Acree, Jr. x ₁	

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.
- 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 \pm 0.1. x_1 : \pm 0.0003.

COMPONENTS:			ORIGINAL MEA	ORIGINAL MEASUREMENTS:			
 Fluorene; Benzene; 	15 10		McLaughlin,	E.	C.P.; Buehring, K.G.;		
VARIABLES:			PREPARED BY:				
Temperature			W.E. Acree,	Jr.			
EXPERIMENTAL V	ALUES			-			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>×</i> 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					

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 \pm 0.1. x_1 : \pm 0.0003.

COMPONENTS:

- (1) Fluorene; C₁₃H₁₀; [86-73-7]
- (2) Benzene; C₆H₆; [71-43-2]

EVALUATOR:

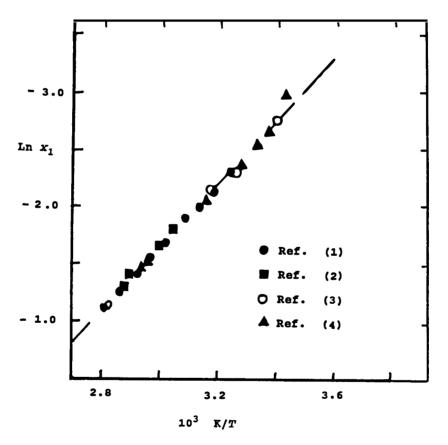
W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
August, 1994

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 $\operatorname{Ln} x_1$ versus 1/T yielded the following mathematical relationship:

In $x_1 = -2668.6 (1/T) + 6.8891$ (r = 0.9995) for variation of fluorene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

- Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.
- 2. McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1959, 863-867.
- 3. Mortimer, F.S. J. Am. Chem. Soc. 1923, 45, 633-641.
- Domanska, U.; Groves, F.R., Jr.; McLaughlin, E. J. Chem. Eng. Data 1993, 38, 88-94.

					•			
COMPONENTS:			ORIGINAL MEASUREMENTS:					
(1) Fluorene	; C ₁₃ H ₁₀ ; [86-	73-7]	McLaughl	McLaughlin, E.; Zainal, H.A.				
(2) Benzene;	C ₆ H ₆ ; [71-43-	-2]	J. Chem.	Soc. 1959,	863-867.			
VARIABLES:			PREPARED I	BY:				
Temperature			W.E. Acre	ee, Jr.				
EXPERIMENTAL V	VALUES							
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	N .				
METHOD: APPARI	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:			
thermometer.		and a precision	(1) Purity not specified, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene eluant.					
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			(2) "AnalaR", was dried over sodium wire and freshly distilled before use.					
	emperature at	which the last	ESTIMATED	ERRORS:				
	30000 410	-FF	T/K: pred x ₁ : ± 0.0	cision \pm 0.1. 0003 (compile	r).			

(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Benzene; C ₆ H ₆ ; [71-43-2]			ORIGINAL	ORIGINAL MEASUREMENTS:				
			Mortime	Mortimer, F.S.				
			J. Am. (Chem. Soc. <u>1</u>	<u>923</u> , <i>45</i> , 633-641.			
VĀRIABLES:			PREPARED	BY:				
Temperature			W.E. Act	ree, Jr.				
EIPERIMENTAL	VALUES							
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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						

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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS:		ORIGINAL MEA	SUREMENTS:			
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Benzene; C ₆ H ₆ ; [71-43-2]		E.				
			g. Data <u>1993</u> , 38, 88-94.			
VARIABLES:		PREPARED BY:				
Temperature	Temperature		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)			

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer. $% \left(1\right) =\left(1\right) \left(1\right)$

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 \pm 0.1. x_1 : \pm 0.0003.

COMPONENTS:	OMPONENTS: (1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]		ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Fluoren			Mortime	r, F.S.			
(2) Methylbenzene; C ₇ H ₈ ; [108-88-3]		J. Am. (Chem. Soc. 1	9 <u>23</u> , <i>45</i> , 633-641.			
ARIABLES:			PREPARED	BY:			
Temperature			W.E. Ac	ree, Jr.			
EXPERIMENTAL	VALUES						
T/K	<i>x</i> ₂	<i>x</i> 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					

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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS:	PONENTS:			ORIGINAL MEASUREMENTS:			
(1) Fluorene	; C ₁₃ H ₁₀ ; [86-	73-7]	Coon, J.	E.; Auwaerte:	r, J.E.; McLaughlin, E.		
	Tetrahydronar 119-64-2]	ohthalene;	Fluid Ph	ase Equilibr.	<u>1989</u> , 44, 305-345.		
VARIABLES:			PREPARED	BY:			
Temperature			W.E. Acr	ee, Jr.			
EXPERIMENTAL	VALUES						
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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 \pm 0.1. x_1 : \pm 0.0003.

COMPONENTS: ORIGINAL MEASUREMENTS: Kravchenko, V.M. (1) Fluorene; C₁₃H₁₀; [86-73-7] J. Appl. Chem. U.S.S.R. 1952, 25, 1015-1022. (English translation) (2) Ethylbenzene; C₈H₁₀; [100-41-4] VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES Solid Phase T/K x_2 x₁ 1.000 0.000 178.8 (2) 0.010 Eutectic 178.2 0.990 209.2 0.979 0.021 (1) 253.2 0.951 0.046 (1) 0.900 281.8 0.100 (1) 308.4 0.801 0.199 (1) 0.702 0.298 (1) 325.9 339.0 0.602 0.398 (1) 0.498 0.502 (1) 349.2 357.2 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:

- 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:

				4
COMPONENTS:		ORIGINAL ME	asurements:	
(1) Fluorene; C ₁₃ H ₁₀ ;	[86-73-7]	Kravchenko	o, V.M.	
(2) 1,3-Dimethylbenz [108-38-3]			them. U.S.S.R. 1952, 25, 1015- lish translation)	
VARIABLES:		PREPARED BY	(1	
Temperature		W.E. Acree	e, Jr.	
EXPERIMENTAL VALUES				
T/K	x ₂	<i>x</i> 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)	

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

1.000

0.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

387.2

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.

(1)

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

ESTIMATED ERRORS:

COMPONENTS:	omponents:		ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Fluoren	e; C ₁₃ H ₁₀ ; [86	-73-7]	Mortime	r, F.S.			
(2) 1,4-Dimethylbenzene; C ₈ H ₁₀ ; [106-42-3]		J. Am. Chem. Soc. 1923, 45, 633-641					
ARIABLES:		PREPARED	BY:				
Temperature			W.E. Ac	W.E. Acree, Jr.			
IPERIMENTAL	1127 1170						
			- 414				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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					

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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

nenko, V.M.
ol. Chem. U.S.S.R. <u>1952</u> , 25, 1015- (English translation)
D BY:
cree, Jr.
A

EXPERIMENTAL VALUES		,		
T/K	x ₂	<i>x</i> 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:

- 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:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kravchenko, V.M. J. Appl. Chem. U.S.S.R. 1952, 25, 1015-(2) Naphthalene; C₁₀H₈; [91-20-3] 1022. (English translation) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₁ x2 1.000 0.000 353.2 (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 0.388 0.612 (1) 337.0 0.436 0.564 (1) 348.7 0.466 0.534 (1) 0.641 358.6 0.359 (1) 0.753 368.5 0.247 (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:

- 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:

(1) Fluorene; C₁₃H₁₀; [86-73-7] (2) 2-Methylnaphthalene; C₁₁H₁₀; [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.

EIPERIMENTAL VALUES

T/K	x ₂	<i>x</i> 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:

- 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:

COMPONENTS: (1) Fluoren

(1) Fluorene; C₁₃H₁₀; [86-73-7]

(2) 2,7-Dimethylnaphthalene; C₁₂H₁₂; [582-16-1]

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	<i>x</i> 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)
	370.2 361.6 352.7 347.7 343.0 337.7 335.2 338.2 342.7 348.3 353.7 363.8 371.7 379.7	370.2 1.000 361.6 0.864 352.7 0.740 347.7 0.689 343.0 0.642 337.7 0.599 335.2 0.580 338.2 0.547 342.7 0.500 348.3 0.444 353.7 0.397 363.8 0.295 371.7 0.198 379.7 0.100	370.2 1.000 0.000 361.6 0.864 0.136 352.7 0.740 0.260 347.7 0.689 0.311 343.0 0.642 0.358 337.7 0.599 0.401 335.2 0.580 0.420 338.2 0.547 0.453 342.7 0.500 0.500 348.3 0.444 0.556 353.7 0.397 0.603 363.8 0.295 0.705 371.7 0.198 0.802 379.7 0.100 0.900

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

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:

- 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:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kravchenko, V.M.; Pastukhova, I.S. J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (2) Fluoranthene; C₁₆H₁₀; [206-44-0] (English translation) PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K **x**₁ $\boldsymbol{x_2}$ 1.000 0.000 383.2 (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) 0.530 0.470 (2) 343.1 0.481 Eutectic 342.2 0.519 345.3 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)

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

0.901

1.000

0.099

0.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

380.7

387.2

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:

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

(1)

(1)

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

ESTIMATED ERRORS:

Components:		ORIGINAL MEASU	vements:			
(1) Fluorene; (16 ^H 10; [86-73-7]	Kravchenko, V.M.; Pastukhova, I.S.				
(2) Acenaphther	(2) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]		Zhur. Fiz. Khim. 1957, 31, 1802-1811.			
VARIABLES:						
Temperature		W.E. Acree, Jr	· .			
EXPERIMENTAL VA	.ues					
T/K	x ₂	<i>x</i> ₁	Solid Phase			
368.	1.000	0.000	(2)			
361.	0.897	0.103	(2)			
355.0	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.	0.562	0.438	(1)			
348.	0.472	0.528	(1)			
356.0	0.381	0.619	(1)			
367.9	0.254	0.746	(1)			
379.	0.111	0.889	(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:

- 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:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kravchenko, V.M.; Pastukhova, I.S. Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669. (English translation) (2) Chrysene; C₁₈H₁₂; [218-01-9] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₂ **x**₁ 1.000 0.000 528.2 (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 (2) 0.320 0.680 0.205 0.795 419.5 (2) 395.7 0.129 0.871 (2) 0.098 0.902 Eutectic 381.2 384.4 0.052 0.948 (1)

1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

387.2

0.000

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:

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

(1)

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

ESTIMATED ERRORS:

COMPONENTS:	OMPONENTS:		ORIGINAL	MEASUREMENTS:	1	
(1) Fluorene	; C ₁₃ H ₁₀ ; [86-	73-7]	McLaughlin, E.; Zainal, H.A.			
(2) Tetrachloromethane; CCl ₄ ; [56-23-5]		J. Chem. Soc. 1960, 2485-2488.				
VARIABLES:			PREPARED	BY:		
Temperature	Temperature		W.E. Acr	ee, Jr.		
EXPERIMENTAL	VALUES			_		
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> ₁	
311.4	0.8381	0.1619	337.8	0.6564	0.3436	
319.8	0.7931	0.2069				
	0.7501	0.2499				
326.0	0.7501					

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:

- 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 \pm 0.1. x_1 : \pm 0.0003 (compiler).

COMPONENTS:	(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Chlorobenzene; C ₆ H ₅ Cl; [108-90-7]			ORIGINAL MEASUREMENTS: Mortimer, F.S.			
(1) Fluoren							
(2) Chlorob				Chem. Soc. 1	9 <u>23</u> , <i>45</i> , 633-641.		
VARIABLES:			PREPARED	BY:			
Temperature	Temperature		W.E. Ac	ree, Jr.			
EXPERIMENTAL	VALUES						
T/K	<i>x</i> ₂	x ₁	T/K	x ₂	<i>x</i> 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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Fluorene; C ₁₃ H ₁₀ ;	[86-73-7]	Mortimer, F.S.			
(2) Methanol; CH ₄ O;	67-56-1]	J. Am. Chem. Soc. 1923, 45, 633-641.			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES	a				
T/K	<i>x</i> ₂	<i>x</i> 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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ F	I ₁₀ ; [86-73-7]	Mortimer, F.S.
(2) Ethanol; C ₂ H ₆ C	; [64-17-5]	J. Am. Chem. Soc. <u>1923</u> , 45, 633-641.
 VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUE	s	
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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

52 COMPONENTS: ORIGINAL MEASUREMENTS: Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D. (1) Fluorene; C₁₃H₁₀; [86-73-7] (2) 1-Octanol; C₈H₁₈O; [111-87-5] Environ. Sci. Technol. 1985, 19, 522-529. VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(mol dm^{-3})$ t/°C 25.0 0.2082 **AUXILIARY INFORMATION** SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE Highest available commercial purity, specific chemical supplier not given, was used as received. Constant temperature bath, rotator, thermometer, and a gas-liquid chromato-graph with flame ionization detection. Excess solute and solvent placed in (2) 99+ %, Aldrich Chemical Company,

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.

Milwaukee, Wisconsin, USA, was used as

ESTIMATED ERRORS:

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

COMPONENTS:			ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3] VARIABLES: Temperature			Mortime	Mortimer, F.S.			
			J. Am.	Chem. Soc. 1	<u>923</u> , 4 5, 633-641.		
			PREPARED	PREPARED BY:			
			W.E. Ac	W.E. Acree, Jr.			
EXPERIMENTAL	VALUES		<u>.</u>				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>×</i> 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					
		AUXIL	IARY INFORMATIO	ON .			
METHOD: APPAI	RATUS/PROCEDU	RE	SOURCE AL	ND PURITY OF I	MATERIALS:		
		ot given in the		ity and chemi	cal source not giv		

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 equili-brating 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.

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS:	COMPONENTS: (1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]		ORIGINAL	MEASUREMENTS	1		
(1) Fluorene			Choi, P.B.; McLaughlin, E.				
(2) Pyridine	2) Pyridine; C ₅ H ₅ N; [110-86-1]			2) Pyridine; C ₅ H ₅ N; [110-86-1] Ind. Chem. Eng. Fundam. <u>1983</u> , 22, 46-5	Ind. Chem. Eng. Fundam. <u>1983</u> , 22		am. <u>1983</u> , 22, 46-51.
VARIABLES:			PREPARED	BY:			
Temperature	Temperature		W.E. Acr	ee, Jr.			
EXPERIMENTAL '	VALUES						
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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. $% \left(1\right) =\left(1\right) \left(1\right$

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:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.0003.

(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Pyridine; C ₅ H ₅ N; [110-86-1] VARIABLES:			ORIGINAL	ORIGINAL MEASUREMENTS: Mortimer, F.S. J. Am. Chem. Soc. 1923, 45, 633-641.			
			Mortime				
			J. Am.				
			PREPARED BY:				
Temperature		W.E. Ac					
EXPERIMENTAL	VALUES		<u>.</u>				
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS:	COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Aniline; C ₆ H ₇ N; [62-53-3]		Mortimer, F.S. J. Am. Chem. Soc. <u>1923</u> , 45, 633-641.			
					VARIABLES:
Temperature	Temperature		W.E. Acree, Jr.		
EXPERIMENTAL	VALUES				
T/K	x ₂	x ₁	T/K	x ₂	<i>x</i> 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:

- 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: \pm 2 (by compiler). x_1 : \pm 8 % (relative error, by compiler).

COMPONENTS: (1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7] (2) Thiophene; C ₄ H ₄ S; [110-02-1]		ORIGINAL	ORIGINAL MEASUREMENTS: Choi, P.B.; McLaughlin, E. Ind. Chem. Eng. Fundam. 1983, 22, 46-51.		
		Choi, P.			
		Ind. Che			
VARIABLES:			PREPARED 1	BY:	
Temperature		W.E. Acr	W.E. Acree, Jr.		
EXPERIMENTAL '	VALUES				
T/K	<i>x</i> ₂	<i>*</i> 1	T/K	x ₂	<i>x</i> 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 \pm 0.1. x_1 : \pm 0.0003.

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kremann, R. (2) 1,2-Dinitrobenzene; $C_6H_4N_2O_4$; [528-29-0] Monatsch. Chem. 1911, 32, 609-617. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₁ x_2 388.2 1,000 0.000 (2) 0.069 385.0 0.931 (2) 382.8 0.872 0.128 (2) 0.785 378.2 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) 0.607 357.2 0.393 (1)

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

0.701

0.783

0.837

0.886

0.940

1.000

0.299

0.217

0.163

0.114

0.060

0.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

365.2

371.2

375.2

378.2

382.2

385.7

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:

Purity and chemical source were not specified in paper.

(1)

(1)

(1)

(1)

(1)

(1)

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

ESTIMATED ERRORS:

56 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kremann, R. Monatsch. Chem. 1911, 32, 609-617. (2) 1,3-Dinitrobenzene; C₆H₄N₂O₄; [99-65-0] PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K *x*₁ $\boldsymbol{x_2}$ 0.000 362.2 1.000 (2) 0.071 357.7 0.929 (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) 0.370 0.630 356.2 (1) 0.685 0.315 362.7 (1) 365.2 0.260 0.740 (1) 0.152 374.7 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:

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

ESTIMATED ERRORS:

			57	
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]		Kremann, R.		
(2) 1,4-Dinitrobenzene; C ₆ H ₄ N ₂ O ₄ ; [100-25-4]		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 Phas	se :	
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)		

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

1.000

0.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

387.7

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:

 Purity and chemical source were not specified in paper.

(1)

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

ESTIMATED ERRORS:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kremann, R. Monatsch. Chem. 1911, 32, 609-617. (2) 1,3,5-Trinitrobenzene; C₆H₃N₃O₆; [99-35-4] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₂ x_1 394.2 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 0.389 378.2 0.611 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) 0.139 0.861 374.2 (1)379.2 0.076 0.924 (1) 382.2 0.034 0.966 (1) 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

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:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Shinomiya, C. (2) 1,2,3,5-Tetranitrobenzene; J. Chem. Soc. Japan 1940, 15, 259-270. C6H2N4O8; [3698-53-1] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EIPERIMENTAL VALUES Solid Phase T/K x₂ x, 0.000 399.2 1.000 (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

0.398

0.457

0.550

0.728

0.769

0.830

0.914

1.000

1:2 Compound

1:2 Compound

1:2 Compound

1:2 Compound

1:2 Compound

(1)

(1)

(1)

402.7

401.5

397.7

381.2

370.2

373.4

382.2

389.2

0.602

0.543

0.450

0.272

0.231

0.170

0.086

0.000

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 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). x₁: ± 0.002 (Compiler).

COMPONENTS:

- (1) Fluorene; C₁₃H₁₀; [86-73-7]
- (2) 2,4-Dinitro-1-methylbenzene; C₇H₆N₂O₄; [121-14-2]

ORIGINAL MEASUREMENTS:

Kremann, R.

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

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x ₂	<i>x</i> 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/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	x ₂	<i>x</i> 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-tri-nitromethylbenzene 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

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:

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

ESTIMATED ERRORS:

62 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] Kremann, R. Monatsch. Chem. 1911, 32, 609-617. (2) 2,4-Dinitrophenol; C₆H₄N₂O₅; [51-28-5] PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES Solid Phase T/K x₁ \mathbf{x}_{2} 0.000 385.2 1.000 (2) 378.2 0.872 0.128 (2) 0.225 (2) 373.2 0.775 368.7 0.711 0.289 (2) 0.340 365.2 0.660 (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) 0.466 348.2 0.534 (2) Eutectic 347.2 0.455 0.545 349.2 0.431 0.569 (1) 0.427 0.573 350.7 (1) 352.2 0.409 0.591 (1) 355.7 0.376 0.624 (1) 363.2 0.304 0.696 (1) 0.823 375.2 0.177 (1) 0.000 1.000 385.7 (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:

COMPONENTS: (1) Fluorene; C₁₃H₁₀; [86-73-7] (2) 2,4,6-Trinitrophenol; C₆H₃N₃O₇; [88-89-1] VARIABLES: Temperature ORIGINAL MEASUREMENTS: Kremann, R. Monatsch. Chem. 1911, 32, 609-617. PREPARED BY: W.E. Acree, Jr.

MENTAL 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

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:

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

ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	Efremov, N.N.; Fikhomirova, A.N.
(2) 6-Methyl-2,3,4-trinitrophenol; C ₇ H ₅ N ₃ O ₇ ; [89793-90-8]	J. Russ. Phys. Chem. Soc. <u>1927</u> , 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	SOURCE AND PURITY OF MATERIALS:			
Experimental details not given in paper. determined using a Toshiniwal Melting Point Apparatus equipped with a precision thermometer.	(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. <u>Esters</u>
- E. Ethers

diphenyl ether

- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. Alcohols

ethanol

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

quinoline 2-methylindole 5-methylindole

J. Binary Solvent Mixtures

COMPONENTS: (1) Indole; C₈H₇N; [120-72-9] (2) Benzene; C₆H₆; [71-43-2] VARIABLES: Temperature ORIGINAL MEASUREMENTS: Yokoyama, C.; Ebina, T.; Takahashi, S. J. Chem. Eng. Data 1993, 38, 583-586. PREPARED BY: W.E. Acree, Jr.

EXPERIMENTAL VALUES			
T/K	* 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)

0.0000

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

1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

326.26

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.

(1)

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

ESTIMATED ERRORS:

T/K: precision \pm 0.02. x_1 : \pm 0.0001.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Indole; C ₈ H ₇ N; [120-72-9]	Yokoyama, C.; Ebina, T.; Takahashi, S.
(2) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	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	
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:

- 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 \pm 0.02. x_1 : \pm 0.0001.

COMPONENTS: ORIGINAL MEASUREMENTS: Szafranski, A.M.; Wyrzykowska-Stankiewicz, (1) Indole; C_RH₇N; [120-72-9] (2) Biphenyl; C₁₂H₁₀; [92-52-4] Int. DATA Ser., Ser. A 1984, 46. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x2 1.0000 0.0000 (2) 341.99 0.1027 (2) 337.00 0.8973 0.1276 335.75 0.8724 (2) 0.8356 0.1644 (2) 333.90 329.75 0.7524 0.2476 (2) 323.85 0.6393 0.3607 (2) 0.5326 0.4674 317.65 (2) 0.5683 310.95 0.4317 (2) 302.70 0.3362 0.6638 (2) 0.3055 0.6945 302.05 (1) 0.7544 306.45 0.2456 (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:

- 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 \pm 0.1. x_1 : \pm 0.0005.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Indole; C₈H₇N; [120-72-9] Yokoyama, C.; Ebina, T.; Takahashi, S. J. Chem. Eng. Data 1993, 38, 583-586. (2) 1-Methylnaphthalene; C11H10; [90-12-0] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EIPERIMENTAL VALUES Solid Phase T/K **x**₂ x₁ 242.45 1.0000 0.0000 (2) 0.0340 239.55 0.9660 (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)

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

1.0000

0.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

326.26

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, Mil-waukee, Wisconsin, USA, was used as received.

(1)

(2) 99.9 %, Aldrich Chemical Comapny, was dried over molecular sieves prior to

ESTIMATED ERRORS:

T/K: precision \pm 0.02. x_1 : \pm 0.0001.

ORIGINAL MEASUREMENTS: COMPONENTS: Yokoyama, C.; Ebina, T.; Takahashi, S. (1) Indole; C₈H₇N; [120-72-9] (2) 2-Methylnaphthalene; C₁₁H₁₀; [91-57-6] J. Chem. Eng. Data 1993, 38, 583-586. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₂ x₁ 1.0000 0.0000 307.09 (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)

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

1.0000

0.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

326.26

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.

(1)

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

ESTIMATED ERRORS:

T/K: precision \pm 0.02. x_1 : \pm 0.0001.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Indole; CgH7N; [120-72-9] Szafranski, A.M.; Wyrzykowska-Stankiewicz, (2) 2-Methylnaphthalene; C11H10; [91-57-6] Int. DATA Ser., Ser. A 1984, 48. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K $\boldsymbol{x_2}$ X₁ 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)

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

0.7391

0.8292

0.9161

1.0000

0.2609

0.1708

0.0839

0.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

305.55

311.95

318.35

324.95

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:

Pure Grade, Inst. Chem. Przerobki Wegla, Zabrze, Poland, was recrystal-lized thrice from aqueous-methanol.

(1)

(1)

(1)

(1)

(2) Pure Grade, Inst. Chem. Przerobki Wegla, was recrystallized thrice from methanol.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : ± 0.0005.

COMPONENTS: (1) Indole; C ₈ H ₇ N; [120-72-9] (2) 2,6-Dimethylnaphthalene; C ₁₂ H ₁₂ ; [581-42-0]] VARIABLES: Temperature		Szafranski, D. Int. DATA S PREPARED BY:	Int. DATA Ser., Ser. A 1984, 49.	
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. = (0.8900 and T/K = 316.15.	

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:

 x_1 : \pm 0.0005.

COMPONENTS: (1) Indole; C₈H₇N; [120-72-9] (2) Diphenyl ether; C₁₂H₁₀O; [101-84-8] VARIABLES: Temperature ORIGINAL MEASUREMENTS: Szafranski, A.M.; Wyrzykowska-Stankiewicz, D. Int. DATA Ser., Ser. A 1984, 50. PREPARED BY: W.E. Acree, Jr.

T/K x2 x1 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)	EXPERIMENTAL VALUES		•	
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)	T/K	x ₂	<i>x</i> ₁	Solid Phase
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)	300.00	1.0000	0.0000	(2)
289.05	294.15	0.8610	0.1390	(2)
283.75	291.55	0.7959	0.2041	(2)
282.35	289.05	0.7336	0.2664	(2)
281.75	283.75	0.6163	0.3837	(2)
286.15	282.35	0.5884	0.4116	(2)
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)	281.75	0.5611	0.4389	(1)
301.15	286.15	0.5080	0.4920	(1)
307.95 0.2278 0.7722 (1) 313.85 0.1468 0.8532 (1)	294.55	0.4077	0.5923	(1)
313.85 0.1468 0.8532 (1)	301.15	0.3145	0.6855	(1)
	307.95	0.2278	0.7722	(1)
324.95 0.0000 1.0000 (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 \pm 0.1. x_1 : \pm 0.0005.

Pucher, G.; Dehn, W.M.
J. Am. Chem. Soc. <u>1921</u> , 43, 1753-1758.
PREPARED BY:
W.E. Acree, Jr.
_

EXPERIMENTAL VALUES

x₂^a x₁^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:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Indole; C ₈ H ₇ N; [120-72-9]	Pucher, G.; Dehn, W.M.		
(2) Quinoline; C ₉ H ₇ N; [91-22-5]	J. Am. Chem. Soc. <u>1921</u> , 43, 1753-1758.		
VARIABLES:	PREPARED BY:		
Ambient Room Temperature	W.E. Acree, Jr.		

EXPERIMENTAL VALUES

x₂^a x₁^a 0.888 0.112

 $^{\rm a}$ 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:

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

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Indole; C₈H₇N; [120-72-9] Yokoyama, C.; Ebina, T.; Takahashi, S. J. Chem. Eng. Data 1993, 38, 583-586. (2) 2-Methylindole; C₀H₀N; [95-20-5] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase *x*₂ x₁ 1.0000 0.0000 332.77 (2) 325.03 0.8875 0.1125 (2) 0.2026 318.87 0.7974 (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)

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

0.7015

0.8001

0.9033

1.0000

0.2985

0.1999

0.0967

0.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

300.39

310.05

318.18

326.26

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:

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

(1)

(1)

(1)

(1)

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

ESTIMATED ERRORS:

T/K: precision \pm 0.02. x_1 : \pm 0.0001.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Indole; C ₈ H ₇ N; [120)-72-9]	Yokoyama, C.; Ebina, T.; Takahashi, S. J. Chem. Eng. Data 1993, 38, 583-586. PREPARED BY: W.E. Acree, Jr.		
(2) 5-Methylindole; C ₉	H ₉ N; [614-96-0]			
ARIABLES:				
Temperature				
XPERIMENTAL VALUES				
T/K	<i>x</i> ₂	<i>x</i> 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 \pm 0.02. x_1 : \pm 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. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthacene; C₁₈H₁₂; [92-24-0] Lissi, E.A.; Abuin, E.B. (2) n-Heptane; C7H16; [142-82-5] Bol. Soc. Chil. Quim. 1981, 26, 19-34. VARIABLES: PREPARED BY: T/K = 293W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(mol dm^{-3})$ t/°C 0.00016 20.0 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, centrifuge, (1) Purity not given, commercial sample of thermometer, and an uv/visible spectrounspecified source, was used as photometer. received. Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. (2) Purity and chemical source not given, purification procedure not specified. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law. ESTIMATED ERRORS:

c1: unknown.

COMPONENTS:	ORIGINAL MEASUREMENTS: Mishra, D.S.; Yalkowsky, S.H.			
(1) Naphthacene; C ₁₈ H ₁₂ ; [92-24-0]				
(2) Benzene; C ₆ H ₆ ; [71-43-2]	Ind. Eng. Chem. Res., <u>1990</u> , 29, 2278-2283.			
VARIABLES:	PREPARED BY:			
T/K = 296	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x ₂	x ₁			
23.0 0.9857	0.0143			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, rotator, thermometer, and an uv/visible spectro-photometer.	 Reagent grade, source not specified, was used as received. 			
Excess solute and solvent placed in screw-capped test tube and allowed to equilibrate for 3 days with gentle agitation in a constant temperature bath. Samples centrifuged for 30 minutes and concentrations were determined spectrophotometrically. Attainment of equilibrium verified by repetitive measurements	(2) Reagent grade, source not specified, was used as received.			
4 days later.	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 ₈ H ₁₈ O; [111-87-5]	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. 1985, 19, 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.

EIPERIMENTAL VALUES

t/°C

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

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 % SE3O ultraphase column.

SOURCE AND PURITY OF MATERIALS:

- 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:

 $T/K: \pm 0.1$ (compiler). $c_1: \pm 3$ % (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
diodomethane
1,1-dibromoethane
1,2-dibromoethane
1,1-dichloroethane
1,2-dichloroethane
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. <u>Ketones</u>

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

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) n-Hexane; C₆H₁₄; [110-54-3]

EVALUATOR:

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

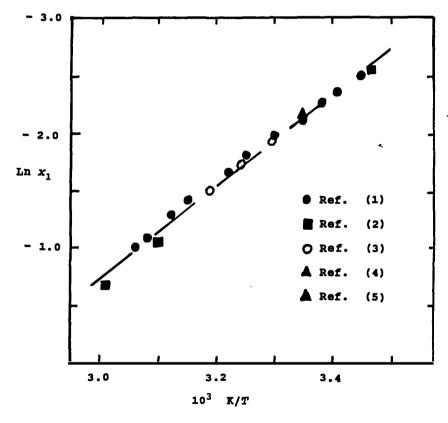
CRITICAL EVALUATION:

Naphthalene solubilities in 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 $\operatorname{Ln} x_1$ versus 1/T yielded the following mathematical relationship:

 $\operatorname{Ln} x_1 = -3849.6 (1/T) + 10.789$ (r = 0.9964)

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



Graphical plot of Ln x_1 versus 1/T

REFERENCES

- Domanska, U. Polish J. Chem. 1981, 55, 1715-1720.
- 2. Ward, H.L. J. Phys. Chem. 1926, 30, 1316-1333.
- 3. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.
- 4. Heric, E.L.; Posey, C.D. J. Chem. Eng. Data 1964, 9, 35-43.
- 5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Heric, E.L.; Posey, C.D.
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	J. Chem. Eng. Data <u>1964</u> , 9, 35-43.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EIPERIMENTAL VALUES		
t/°C	<i>x</i> ₂	<i>x</i> ₁
25.0	0.8832	0.1168
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature and a precision refrac		(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.
Excess solute and solution to the same and allowed to gentle agitation for constant temperature. of saturated solutions solubilities obtained curve. Attainment of	o equilibrate with several days at Refractive indices s were measured and using a calibration	(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.
by making repetitive memory additional day		ESTIMATED ERRORS:
		T/K: precision ± 0.01. x.: precision ± 0.0005.

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Chang, W.
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]	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	<i>x</i> ₂	<i>x</i> ₁
25.0	0.878	0.122
	AUXIL	IARY INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature 1	oath and a precisi	on (1) Purity, source and purification proce-

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.

- dures not specified.
- (2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) n-Hexane; C₆H₁₄; [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	<i>x</i> ₂	<i>x</i> 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:

- 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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

86					
COMPONENTS:			ORIGINAL N	œasurements	•
(1) Naphthale	ene; C ₁₀ H ₈ ; [9	91-20-3]	Ward, H.I	۵.	
(2) n-Hexane	; C ₆ H ₁₄ ; [110-	-54-3]	J. Phys.	Chem. <u>1926</u>	, 30, 1316-1333.
VARIABLES:			PREPARED E	BY:	
Temperature			W.E. Acre	ee, Jr.	
EIPERIMENTAL V	VALUES				
T/K	x ₂	<i>*</i> 1	T/K	× ₂	<i>x</i> 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	ī	
METHOD: APPAR	ATUS/PROCEDUR	RE	SOURCE AND	PURITY OF 1	MATERIALS:
Mixtures of in glass tube temperature tweeter rotated	known concent es and placed to equilibrat while bath t	rations sealed in constant e. Samples emperature slowly termined by visual	recry anol 80.05 (2) Purit Roche	vetallized so to give a mo 5-80.10 °C. Ty not given	e not specified, was everal times from meth- elting temperature of , Eastman Kodak Company ork, USA, was distilled
noting the te	emperature at	which the last	ESTIMATED	ERRORS:	
		times to verify		cision <u>+</u> 0.1. significant	figs. (compiler).

COMPONENTS:			ORIGINAL	MEASUREMENTS:		
	ene; C ₁₀ H ₈ ; [9		Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.			
(2) n-Hexane; C ₆ H ₁₄ ; [110-54-3]		-54-3]	Int. J. Pharm. 1986, 31, 225-230.			
VARIABLES:			PREPARED 1	BY:		
T/K = 303, 3	08 and 313		W.E. Acr	ee, Jr.		
EXPERIMENTAL 1	VALUES					
t/° C	x ₂	<i>*</i> 1	t/° C	<i>x</i> ₂	<i>x</i> ₁	
30.0	0.8585	0.1415	40.0	0.7784	0.2216	
35.0	0.8237	0.1763				
		AUXILIARY	INFORMATION	4		
ETHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
	perature bath and gas chro	, calorimetric matograph.	Milwa		emical Company, nsin, USA, recrystal- m methanol.	
glass bottles for several of Attainment of repetitive me urated soluti	a and allowed days at consta f equilibrium easurements. A lons transfer:	Aliquots of sat- red through a	store		emical Company, was ular sieves and dis- fore use.	
flasks, weigh	centrations de	ed with cyclo-	ESTIMATED T/K: ± 0. x ₁ : ± 1 %		rror).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	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	<i>x</i> ₁
25.0 0.870	0.130
AUXILIARY	INFORMATION
ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	 Purity, source and purification procedures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.
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.	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]		Lissi, E.A.; Abuin, E.B.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]		Bol. Soc. Chil. Quim. <u>1981</u> , 26, 19-34.
VARIABLES:		PREPARED BY:
T/K = 293		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	c ₁ /(mol dm ⁻³)
20.0	0.60)

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 extra-This indirect method computes polates up to saturation point.

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERRORS:

T/K: \pm 2. c1: unknown.

88		
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Chang, W.
(2) n-Octane; C ₈ H ₁₈ ; [111-65-9]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES	<u> </u>	1
t/°C	x ₂	<i>x</i> ₁
25.0	0.858	0.142
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature between thermometer.	eath and a precision	(1) Purity, source and purification procedures not specified.
Mixtures of known cond in glass ampoules and temperature to equilib were rotated while bat increased. Solubility	placed in constant rate. Samples th temperature slowly	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.
noting the temperature trace of solid solute	at which the last disappeared. Sol-	ESTIMATED ERRORS:
ubilities at 298 K int experimental values us 1/T graph.	erpolated from sing ln x ₁ versus	T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).
		1

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ;	[91-20-3]	Heric, E.L.; Posey, C.D.
(2) n-Hexadecane; C ₁₆ H	₃₄ ; [544-76-3]	J. Chem. Eng. Data 1964, 9, 35-43.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		<u> </u>
t/°C	<i>x</i> ₂	<i>x</i> ₁
25.0	0.7957	0.2043
	AUXILIARY	INFORMATION
ŒTHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature b and a precision refrac		(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.
Excess solute and solv bottles and allowed to gentle agitation for s constant temperature. of saturated solutions solubilities obtained curve. Attainment of	equilibrate with everal days at Refractive indices were measured and using a calibration	(2) Practical Grade, Eastman Chemical Company, was dried over phosphorous pentoxide and distilled to a final purity of 99.1 %.
	easurements after	

T/K: precision \pm 0.01. x_1 : precision \pm 0.0005.

						8
COMPONENTS:			ORIGINAL	MEASUREMENTS:	1	
(1) Naphthal	ene; C ₁₀ H ₈ ; [91-20-3]	Djordjev	ic, N.M.		
(2) n-Octade	cane; C ₁₈ H ₃₈ ;	[593-45-3]	Thermoch	im. Acta <u>199</u>	<u>91</u> , <i>177</i> , 109-118.	
VARIABLES:			PREPARED	BY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL '	VALUES		.1			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	1		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
	scanning cal		Compa		, Aldrich Chemica e, Wisconsin, USA	
tration were which were the loss during	weighed into hen crimped t	of known concen- o aluminum pans, o preclude sample process. Solubil-		, Aldrich Che ım-distilled	mical Company, wa before use.	ıS
points of bir	nary mixtures	using a Perkin- scanning calori-	ESTIMATED	ERRORS:		
meter and sca				cision \pm 0.3 0003 (compile		

COMPONENTS:			ORIGINAL	MEASUREMENTS	:
	ene; C ₁₀ H ₈ ; [9 ane; C ₆ H ₁₂ ; [3		C.L.		ntikos, N.M.; Judy,
VARIABLES:			PREPARED	BY:	
T/K = 303, 3	08 and 313		W.E. Acr	ee, Jr.	
			W.E. Acr	ee, Jr.	
		<i>x</i> ₁	W.E. Acr	ee, Jr.	x ₁
EXPERIMENTAL V	/ALUES	x ₁ 0.1825			x ₁ 0.2767

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).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]

EVALUATOR:

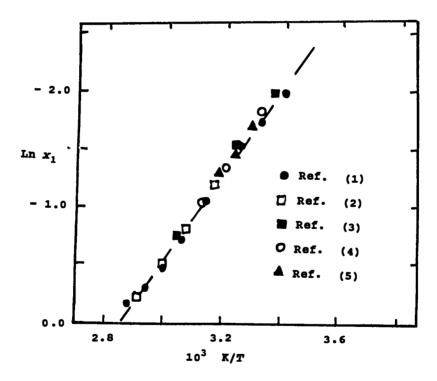
W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas August, 1994 76203-5068 (USA)

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:

 $Ln x_1 = -3916.1 (1/T) + 11.2291$ (r = 0.9984)for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of $Ln x_1$ versus 1/T

REFERENCES

- Heric, E.L.; Yeh, K.-N. J. Chem. Eng. Data 1970, 15, 13-17.
 Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.

 Domanska, U. Polish J. Chem. 1981, 55, 1715-1720.
 McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 3854-3857.
 Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.
 Heric, E.L.; Posey, C.D. J. Chem. Eng. Data 1964, 9, 35-43.
 Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969. 2.
- 4.

	91		
COMPONENTS:	ORIGINAL MEASUREMENTS: Heric, E.L.; Posey, C.D.		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	J. Chem. Eng. Data <u>1964</u> , 9, 35-43.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EIPERIMENTAL VALUES			
t/°C	× ₁		
25.0 0.8513	0.1487		
AUXILIAR	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision refractometer.	(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.		
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	(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 \pm 0.01. x_1 : precision \pm 0.0005.

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		ORIGINAL MEASUREMENTS: Heric, E. L; Yeh, KN. J. Chem. Eng. Data 1970, 15, 13-17.								
					VARIABLES:			PREPARED E	Y:	
					Temperature			W.E. Acre	e, Jr.	
EXPERIMENTAL V	ALUES									
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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.

by making repetitive measurements after several additional days.

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 \pm 0.03. x_1 : \pm 0.0001.

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.			
VARIABLES:	VARIABLES:			Y:	
Temperature		W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES				
T/K	x 2	<i>x</i> ₁	T/K	x 2	<i>x</i> 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: APPARA	rus/Procedur	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.		Roche over talli (2) Gold Compa	ster, New Yo activated al zed from tol Label, 99.9+ ny, was used	odiak Chemical Company, rk, USA, was passed umina and then recrysuene. %, Aldrich Chemical as received.	
		T/K: prec x ₁ : ± 0.00	ision ± 0.1.		

COMPONENTS:			ORIGINAL M	ORIGINAL MEASUREMENTS:		
(1) Naphthale	ene; C ₈ H ₁₀ ; [91-20-3]	Domanska,		. 66 1715-1720	
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		(numerica	Polish J. Chem. 1981, 55, 1715-1720. (numerical values obtained through personal communication with author.)			
VARIABLES:			PREPARED E	PREPARED BY:		
Temperature		W.E. Acre	W.E. Acree, Jr.			
EXPERIMENTAL V	ALUES					
T/K	x ₂	x ₁	T/K	x ₂	<i>x</i> 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				
		AUXILIA	RY INFORMATION			
ŒTHOD: APPARA	ETHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF	MATERIALS:	
Constant temperature bath and a precision thermometer.		Polan	d, was vacu	fied, P.O.Ch., Gliw um sublimed to a		

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.

- melting temperature of 80.25 °C.
- (2) Initial purity not specified, P.O.Ch., was dried over sodium metal and frac-tionally distilled to 99.9+ % purity.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : to 3 significant figs. (compiler).

	Ş
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C × ₂	<i>×</i> 1
25.0 0.853	0.147
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	(1) Purity, source and purification procedures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) Reagent Grade, Eastman Organic Chem- ical, USA, was used as received.
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.	ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 2 % (relative error; compiler).

(1) Naphthalene; C ₁₀ H; [91-20-3] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		ORIGINAL	ORIGINAL MEASUREMENTS:		
		McLaughlin, E.; Zainal, H.A. J. Chem. Soc. <u>1960</u> , 3854-3857.			
					VARIABLES:
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL	VALUES		!		
T/K	x 2	×1	T/K	x ₂	<i>x</i> 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			

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 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:

- 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 \pm 0.1. x_1 : \pm 0.0003 (compiler).

94				
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ;	[91-20-3]	Chang, W.		
(2) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2]		Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	* 2	<i>x</i> ₁		
25.0	0.853	0.147		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature between thermometer.	eath and a precision	(1) Purity, source and purification procedures not specified.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.		
noting the temperature	at which the last	ESTIMATED ERRORS:		
trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.		T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).		

Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969). PREPARED BY:
versity, North Dakota, USA (1969).
PREPARED BY:
W.E. Acree, Jr.
x ₁
0.163
SOURCE AND PURITY OF MATERIALS:
SOURCE AND PURITY OF MATERIALS: (1) Purity, source and purification proce-
dures not specified.
(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.
ESTIMATED ERRORS:
T/K: precision \pm 0.1. x ₁ : \pm 2 % (relative error; compiler).

	9
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.
(2) trans-1,2-Dimethylcyclohexane; C ₈ H ₁₆ ; [6876-23-9]	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	<i>x</i> ₁
25.0 0.847	0.153
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	(1) Purity, source and purification proce- dures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.
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.	T/K: precision ± 0.1. x1: ± 2 % (relative error; compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-2	20-3]	Chang, W.
(2) trans-1,4-Dimethylcycloh C ₈ H ₁₆ ; [2207-04-7]	exane;	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	0.850	0.150
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Constant temperature bath an thermometer.	d a precision	(1) Purity, source and purification procedures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
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.		ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 2 % (relative error; compiler).

	ORIGINAL MEASUREMENTS:		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).		
(2) cis-1,4-Dimethylcyclohexane; C ₈ H ₁₆ ; [624-29-3]			
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES	 		
t/°C x ₂	<i>x</i> ₁		
25.0 0.847	0.153		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	(1) Purity, source and purification procedures not specified.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.		
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.	<pre>ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 2 % (relative error; compiler).</pre>		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) cis-1,3-Dimethylcyclohexane; C ₈ H ₁₆ ; [638-04-0]		Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	x ₂	×1		
25.0	0.845	0.155		
		INFORMATION		
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature ba thermometer.	th and a precision	(1) Purity, source and purification procedures not specified.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by 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.		(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.		
		<pre>T/K: precision ± 0.1. x₁: ± 2 % (relative error; compiler).</pre>		

					9
COMPONENTS:		ORIGINAL)	æasurements:		
 (1) Naphthalene; C₁₀H₈; [91-20-3] (2) Decahydronaphthalene; C₁₀H₁₈; [91-17-8] 		Coon, J.1	E.; Auwaerter	, J.E.; McLaughlin, E.	
		Fluid Phase Equilibr. 1989, 44, 305-345.			
VARIABLES:			PREPARED E	BY:	
Temperature			W.E. Acree, Jr.		
EXPERIMENTAL '	VALUES				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂ .	<i>x</i> 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	Ī	
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.			wauke over then (2) 99+ %	e, Wisconsin an activated recrystallize, Aldrich Cher ratio of 6	hemical Company, Mil- , USA, was passed alumina column and ed from solution. emical Company, having 0.6 % cis and 39.4 % r molecular sieves.
			ESTIMATED	ERRORS:	
			T/K: pred x ₁ : ± 0.00	cision <u>+</u> 0.1.	

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Benzene; C ₆ H ₆ ; [71-43-2]			ORIGINAL	ORIGINAL MEASUREMENTS:			
			C.L.	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.			
VARIABLES:	/ARIABLES: T/K = 303, 308 and 313			PREPARED BY:			
T/K = 303, 3				W.E. Acree, Jr.			
EXPERIMENTAL	VALUES						
t/° C	x ₂	<i>×</i> 1	t/ ⁶ C	<i>x</i> ₂	<i>x</i> ₁		
30.0	0.6682	0.3318	40.0	0.5757	0.4243		
35.0	0.6211	0.3789					
•-		AUXIL:	IARY 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: \pm 0.05. x_1 : \pm 1 % (relative error).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Benzene; C₆H₆; [71-43-2]

EVALUATOR:

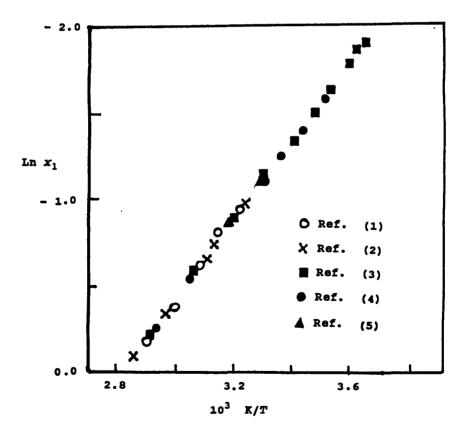
W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
August, 1994

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:

Ln x_1 = -2301.9 (1/T) + 6.5066 (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)

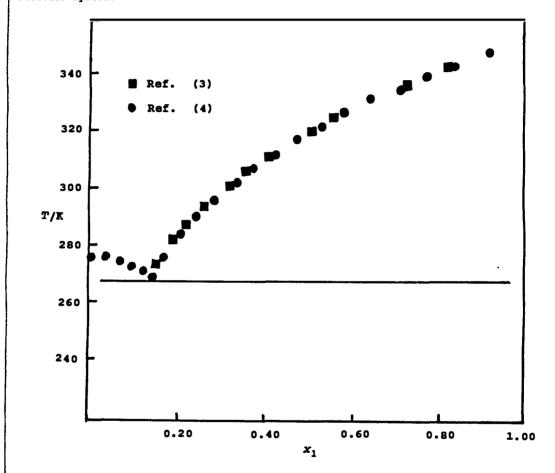
- (1) Naphthalene; C10H8; [91-20-3]
- (2) Benzene; C₆H₆; [71-43-2]

EVALUATOR:

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

- 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.

100						
COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Naphthalene; C ₁₀ H ₈ .	; [91-20-3]	Heric, E.L.; Posey, C.D.				
(2) Benzene; C ₆ H ₆ ; [71	-43-2]	J. Chem. Eng. Data 1964, 9, 35-43.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°c	* 2	<i>x</i> ₁				
25.0 0.7054		0.2946				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature band a precision refrac		(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.				
Excess solute and solve bottles and allowed to gentle agitation for solutions of saturated solutions solubilities obtained curve. Attainment of	o equilibrate with several days at Refractive indices a were measured and using a calibration equilibrium verified	(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over metallic sodium distilled to a final purity of 99.95 %.				
by making repetitive meseveral additional day		ESTIMATED ERRORS:				
		T/K : precision \pm 0.01. x_1 : precision \pm 0.0005.				

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Benzene; C ₆ H ₆ ; [71-43-2]			ORIGINAL MEASUREMENTS:			
			Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.			
VARIABLES:			PREPARED B	Y:		
Temperature			W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES		!			
T/K	<i>x</i> ₂	x ₁	T/K	x ₂	<i>x</i> 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: APPARA	TUS/PROCEDUR	3	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			 (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. 			
increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.			T/K: prec x ₁ : ± 0.00	ision ± 0.1.		

	101
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.
(2) Benzene; C ₆ H ₆ ; [71-43-2]	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 0.708	0.292
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	 Purity, source and purification procedures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) Spectroanalyzed, Eastman Organic Chemical Company, USA, was used as received.
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.	<pre>ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 2 % (relative error; compiler).</pre>

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Benzene; C ₆ H ₆ ; [71-43-2] VARIABLES: Temperature			ORIGINAL MEASUREMENTS: McLaughlin, E.; Zainal, H.A.			
			PREPARED BY:			
			W.E. Acre	ee, Jr.		
			XPERIMENTAL '	VALUES		
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	¥		
ETHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.						
						ESTIMATED
				cision <u>+</u> 0.1.		

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Benzene; C₆H₆; [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	<i>x</i> 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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

COMPONENTS:		ORIGINAL ME	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Benzene; C ₆ H ₆ ; [71-43-2]		Kravchenko	Kravchenko, V.M.		
		Zhur. Fiz.	Zhur. Fiz. Khim. 1939, 13, 133-145.		
VARIABLES:		PREPARED BY	1		
Temperature		W.E. Acree	, Jr.		
EIPERIMENTAL VALUES					
т/к	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:

- 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Methylbenzene; C7H8; [108-88-3]

EVALUATOR:

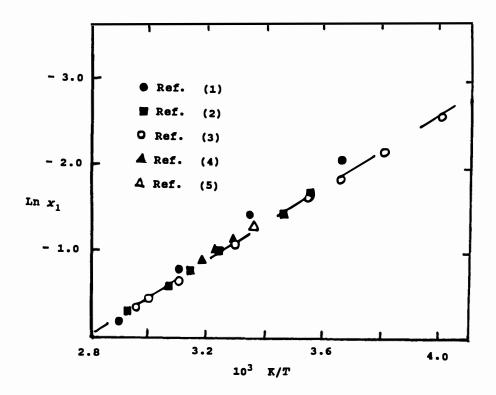
W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas August, 1994 76203-5068 (USA)

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:

 $Ln x_1 = -1870.2 (1/T) + 5.0916$ (r = 0.9839)for variation of naphthalene solubility with absolute temperature (see graph below).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

- 2.
- Speyers, C.L. Am. J. Sci. 1902, 14, 293-302. Ward, H.L. J. Phys. Chem. 1926, 30, 1316-1333. Kravchenko, V.M. Zhur. Fiz. Khim. 1939, 13, 133-145. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. Heric, E.L.; Posey, C.D. J. Chem. Eng. Data 1964, 9, 35-43. 3. <u>1986</u>, 31, 225-230.
- 5.
- Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

			10			
COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Heric, E.L.; Posey, C.D.				
(2) Methylbenzene; C ₇ H ₈ ; [108-88-3]		J. Chem. Eng. Data <u>1964</u> , 9, 35-43.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°C	* ₂	x ₁				
25.0 0.7080		0.2920				

AUXILIARY	AUXILIARY INFORMATION								
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:								
Constant temperature bath, thermometer, and a precision refractometer.	(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.								
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.	(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 \pm 0.01. x_1 : precision \pm 0.0005.								

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Chang, W.		
(2) Methylbenzene; C ₇ H	8; [108-88-3]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).		
VARIABLES:	RIABLES: PREPARED BY:			
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		,		
t/°C	x ₂	x ₁		
25.0 0.708		0.292		
-	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
MEIROD: AFFARAIUS/FRUCE				

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 x₁ versus 1/T graph. (2) Reagent Grade, Eastman Organic Chem-ical, USA, was used as received. ESTIMATED ERRORS: T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

106						
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3]		ORIGINAL MEASUREMENTS: Ward, H.L.				
						J. Phys.
		VARIABLES:			PREPARED I	BY:
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL	VALUES		_			
T/K	<i>x</i> ₂	<i>*</i> 1	T/K	<i>x</i> ₂	<i>x</i> 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	7		
METHOD: APPAR	ATUS/PROCEDUI	RE	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			 (1) Purity and source not specified, was recrystallized several times from meth anol to give a melting temperature of 80.05-80.10 °C. (2) Analyzed Grade, source not given, was fractionally distilled before use. 			
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.				cision + 0.1	figs. (compiler).	

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3] VARIABLES: Temperature			ORIGINAL	ORIGINAL MEASUREMENTS: Speyers, C.L. Am. J. Sci. 1902, 14, 293-302. PREPARED BY:			
			Speyers,				
			Am. J. S				
			PREPARED				
			W.E. Acr	W.E. Acree, Jr.			
EXPERIMENTAL	VALUES						
T/K	*2	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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					
		AUXILIA	RY INFORMATION	N			
ETHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	MATERIALS:		
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant			tall	(1) Purity not given, Kahlbaum, was recrys- tallized from alcohol to a melting point temperature of 80.1 °C.			

temperature water bath for between 10-30 minutes. Saturated solution was with-

drawn 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.

ESTIMATED ERRORS:

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

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

OPICINAL MEASUREMENTS! COMPONENTS: Kravchenko, V.M. (1) Naphthalene; C₁₀H₈; [91-20-3] Zhur. Fiz. Khim. 1939, 13, 133-145. (2) Methylbenzene; C7H8; [108-88-3] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K *x*₂ x₁ 0.988 0.012 177.7 (2) 0.978 0.022 Eutectic 177.2 188.2 0.975 0.025 (1) 0.029 200.7 0.971 (1) 0.037 214.2 0.963 (1) 0.956 0.044 217.7 (1) 0.052 227.1 0.948 (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) 0.483 0.517 321.4 (1) 331.2 0.373 0.627 (1) 338.2 0.256 0.744 (1)

Author reports eutectic point occurs at $x_1 = 0.022$ and T/K = 177.2.

0.879

0.121

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

346.4

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.

(1)

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

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:								
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methylbenzene; C ₇ H ₈ ; [108-88-3] VARIABLES: T/K = 303, 308 and 313		Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230. PREPARED BY: W.E. Acree, Jr.								
					EXPERIMENTAL '	VALUES	<u></u>	•		
					t/° C	<i>x</i> ₂	<i>x</i> ₁	t/° C	<i>x</i> ₂	<i>x</i> ₁
30.0	0.6709	0.3291	40.0	0.5784	0.4216					
35.0	0.6289	0.3711								
		AUXILIARY	INFORMATION	I						
METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:						
Constant temperature bath, calorimetric thermometer, and gas chromatograph.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.								
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a		(2) Gold Label, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.								
coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined chromatographically.		ESTIMATED ERRORS: T/K: ± 0.05. x.: + 1 % (relative error).								

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Heric, E.L.; Posey, C.D.
(2) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	J. Chem. Eng. Data <u>1964</u> , 9, 35-43.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	-
t/°C	× ₁
25.0 0.7074	0.2926
A	UXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermome and a precision refractometer.	ter, (1) Eastman Chemical Company, Rochester, New York, USA, was used as received.
Excess solute and solvent placed in bottles and allowed to equilibrate gentle agitation for several days a constant temperature. Refractive in of saturated solutions were measure solubilities obtained using a calib curve. Attainment of equilibrium v	with USA, was dried over calcium hydride and t distilled to a final purity of 99.8 %. dd and dration erified
by making repetitive measurements a several additional days.	fter ESTIMATED ERRORS:
	T/K : precision \pm 0.01. x_1 : precision \pm 0.0005.

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Ethylbenzene; C₈H₁₀; [100-41-4]

EVALUATOR:

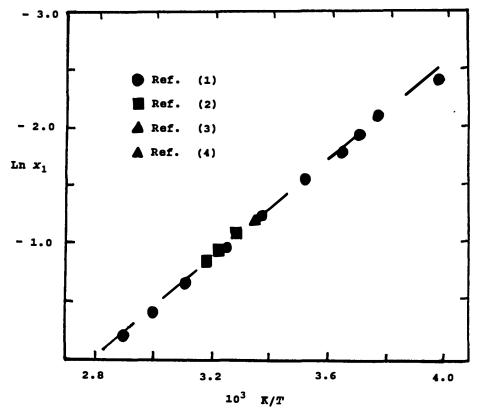
W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
August, 1994

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:

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.
- Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

GINAL MEASUREMENTS: ang, W. .D Dissertation, North Dakota State Unirisity, North Dakota, USA (1969). PARED BY: E. Acree, Jr.
D Dissertation, North Dakota State Unirisity, North Dakota, USA (1969). PARED BY: E. Acree, Jr.
rsity, North Dakota, USA (1969). PARED BY: E. Acree, Jr.
E. Acree, Jr.
289
RMATION
RCE AND PURITY OF MATERIALS:
Purity, source and purification procedures not specified.
Reagent Grade, Eastman Organic Chemical, USA, was used as received.
MATED ERRORS:
K: precision + 0.1.
1

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Ethylbenzene; C ₈ H ₁₀ ; [100-14-4] VARIABLES: T/K = 303, 308 and 313			Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230. PREPARED BY:			
						W.E. Acree, Jr.
			EXPERIMENTAL V	/ALUES		
t/º C	x ₂	<i>x</i> ₁	t/° C	x ₂	<i>x</i> ₁	
30.0	0.6712	0.3288	40.0	0.5767	0.4233	
35.0	0.6295	0.3705				
			INFORMATION			
METHOD: APPARATUS/PROCEDURE Constant temperature bath, calorimetric thermometer, and gas chromatograph.			SOURCE AND PURITY OF MATERIALS: (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a			(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.			
coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined chromatographically.			ESTIMATED ERRORS: T/K : \pm 0.05. x_1 : \pm 1 % (relative error).			

Components:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Kravchenko, V.M.		
(2) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Zhur. Priklad. Khim. 1949, 22, 724-733.		
VARIABLES:	PREPARED BY:		
Temperature	W.E. Acree, Jr.		

IMENTAL VALUES		·		
T/K	x ₂	<i>x</i> 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:

- 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: Kravchenko, V.M. (1) Naphthalene; C₁₀H₈; [91-20-3] (2) 1,2-Dimethylbenzene; C₈H₁₀; [95-47-6] Zhur. Priklad. Khim. 1949, 22, 724-733. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES x₂ Solid Phase T/K $\boldsymbol{x_1}$ 247.7 1.000 0.000 (2) 0.963 0.037 246.2 (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) 0.848 272.7 0.152 (1) 0.203 282.7 0.797 (1) 0.689 0.311 298.7 (1) 309.2 0.406 0.594 (1) (1) 313.9 0.548 0.452 318.5 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) 0.103 0.897 346.4 (1) 0.000 1.000 353.2 (1) AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Phase diagram was determined using a (1) Purity and chemical source were not specified in paper, was recrystallized thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. 1939, 13, 133), supplemented by visual observations. before use. (2) Purity and chemical source were not specified in paper, was distilled before use. ESTIMATED ERRORS: T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Kravchenko, V.M.
(2) 1,3-Dimethylbenzene; C ₈ H ₁₀ ; [108-38-3]	Zhur. Fiz. Khim. <u>1939</u> , 13, 989-1000.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES						
T/K	x ₂	× 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:

- 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

114 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; $C_{10}H_8$; [91-20-3] Kravchenko, V.M. (2) 1,4-Dimethylbenzene; C₈H₁₀; [106-42-3] Zhur. Priklad. Khim. 1949, 22, 724-733. VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K Solid Phase x₁ x_2 0.000 1.000 (2) 286.5 (2) 0.051 283.8 0.949 0.893 0.107 (2) 281.2 0.150 279.2 0.850 (2) 277.4 0.818 0.182 Eutectic 281.2 0.799 0.201 (1) 0.254 290.5 0.746 (1) 0.698 0.302 297.2 (1) 0.590 0.410 310.2 (1) 318.4 0.497 0.503 (1) 0.594 0.406 (1) 325.0 0.299 0.701 333.2 (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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Lee, H.H.; Warner, J.C. J. Am. Chem. Soc. 1935, 57, 318-321. (2) Biphenyl; C₁₂H₁₀; [92-52-4] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K x₂ Solid Phase x_1 342.2 1.000 0.000 (2) 336.7 0.898 0.102 (2) 0.806 0.194 331.0 (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) 0.449 0.551 322.8 (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) 0.000 353.3 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 \pm 0.1. x_1 : ± 0.001.

116 ORIGINAL MEASUREMENTS: COMPONENTS: Lee, H.H.; Warner, J.C. (1) Naphthalene; C10H8; [91-20-3] J. Am. Chem. Soc. 1935, 57, 318-321. (2) 1,2-Diphenylethane; C₁₄H₁₄; [103-29-7] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₁ *x*₂ 0.000 1.000 (2) 324.5 (2) 320.2 0.900 0.100 0.201 0.799 (2) 315.5 0.701 0.299 (2) 310.7 307.9 0.649 0.351 (2) 0.620 0.380 (2) 306.1 Eutectic 305.7 0.614 0.386 0.390 306.2 0.610 (1) 0.420 309.7 0.580 (1) 318.6 0.490 0.510 (1) 327.1 0.390 0.610 (1) 339.6 0.772 0.228 (1) 0.199 0.801 (1) 341.3 353.3 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 \pm 0.1. x_1 : ± 0.001.

COMPONENTS:			ORIGINAL I	measurements:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Coon, J.1	E.; Auwaerter	, J.E.; McLaughlin, E.	
(2) 1,2,3,4-Tetrahydronaphthalene; C ₁₀ H ₁₂ ; [119-64-2]			Fluid Phase Equilibr. 1989, 44, 305-345.			
VARIABLES:			PREPARED I	BY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL V	VALUES		!			
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	INFORMATIO	N		
METHOD: APPARI	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			(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.			
						noting the te
trace of solid solute disappeared.			T/K: pred x ₁ : ± 0.0	cision <u>+</u> 0.1.		

ORIGINAL MEASUREMENTS:
Wheeler, A.S.
J. Am. Chem. Soc. 1920, 42, 1842-1846.
PREPARED BY:
W.E. Acree, Jr.
×1
0.1296
AUXILIARY INFORMATION
SOURCE AND PURITY OF MATERIALS:
eter, (1) Purity and source not given.
(2) Purity and source not given.
n closed
t ed solu-
iners ted from ESTIMATED ERRORS:
ined
T/K : precision \pm 0.5 (compiler). x_1 : \pm 5 % (relative error; compiler).

COMPONENTS:		ORIGINAL MEAS	GUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Kravchenko, V.M.; Pastukhova, I.S.			
(2) Indene; C ₉ H ₈ ; [95-	13-6]	J. Appl. Chem. U.S.S.R. <u>1952</u> , 25, 343-350. (English translation)			
ARIABLES:		PREPARED BY:			
Temperature		W.E. Acree,	Jr.		
EXPERIMENTAL VALUES ^a					
$oldsymbol{ au_{in}}/\kappa$	T_{fin}/K	<i>x</i> ₂	<i>x</i> 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		

⁸ 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. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ 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:

- 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Kravchenko, V.M.; Pastukhova, I.S. (2) Fluoranthene; C₁₆H₁₀; [206-44-0] J. Gen. Chem. U.S.S.R. 1959, 29, 29-34. (English translation) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EIPERIMENTAL VALUES Solid Phase T/K x_2 x₁ 383.2 1.000 0.000 (2) 374.2 0.875 0.125 (2) 361.4 0.707 0.293 (2) 0.614 0.386 352.8 (2) 0.519 343.5 0.471 (2) 337.1 0.461 0.539 (2) 330.9 0.411 0.589 (2) 329.0 0.390 0.610 Eutectic

Authors report eutectic point occurs at $x_2 = 0.390$ and at T/K = 329.0.

0.663

0.753

0.883

1.000

0.337

0.247

0.117

0.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

332.2

338.5

346.3

353.4

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:

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

(1)

(1)

(1)

(1)

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

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL ME	ORIGINAL MEASUREMENTS: Kravchenko, V.M. J. Appl. Chem. U.S.S.R. 1952, 25, 1015-1022. (English translation)		
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Kravchenko			
(2) Fluorene; C ₁₃ H ₁₀ ;	[86-73-7]	J. Appl. C 1022. (Eng			
VARIABLES:		PREPARED BY	:		
Temperature		W.E. Acree	W.E. Acree, Jr.		
EXPERIMENTAL VALUES					
T/K	x ₂	<i>x</i> 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

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). x1: ± 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: Kravchenko, V.M.; Pastukhova, I.S. (1) Naphthalene; C₁₀H₈; [91-20-3] Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669. (English translation) (2) Chrysene; C₁₈H₁₂; [218-01-9] PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K ×₁ x_2 0.000 528.2 1.000 (2) 520.2 0.903 0.097 (2) 511.4 0.817 0.183 (2) 0.298 500.2 0.702 (2) 487.5 0.407 (2) 0.593 476.2 0.504 0.496 (2) 459.7 0.407 0.593 (2) 442.4 0.290 0.710 (2) 0.202 0.798 417.8 (2) 406.2 0.157 0.843 (2) 388.4 0.103 0.897 (2) 351.0 0.042 0.958 Eutectic 0.975 351.7 0.025 (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:

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	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.

EIPERIMENTAL 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.

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. ESTIMATED ERRORS: T/K: precision ± 0.3 (Compiler). x1: ± 0.02 (Compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]			ORIGINAL MEASUREMENTS:				
			Kravchenko, V.	M.; Pastukho	va, I.S.		
			Zhur. Fiz. Khi	m. <u>1957</u> , <i>31</i>	, 1802-1811.		
VARIABLES:			PREPARED BY:				
Temperature			W.E. Acree, Jr	•			
IPERIMENTAL '	VALUES						
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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				
ŒTHOD: APPARI	ATUS/PROCEDUI	Œ	SOURCE AND PURI	TY OF MATERIA	ALS:		
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 specified		urce were not		
			(2) Purity and specified		erce were not		

ESTIMATED ERRORS:

 x_1 : \pm 0.002 (Compiler).

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

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		ORIGINAL MEASUREMENTS:
		Sunier, A.A.
(2) Furfuryl Acetate; [623-17-6]	C7H8O3;	J. Phys. Chem. <u>1931</u> , 35, 1756-1761.
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		<u> </u>
T/K	x ₂	× 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. $% \left(1\right) =\left(1\right) \left(1\right$

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:

- 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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

results.

METHOD: APPARATUS/PROCEDURE

thermometer.

results.

Constant temperature bath and a precision

Mixtures of known concentrations sealed

were rotated while bath temperature slowly

trace of solid solute disappeared. Meas-

urements repeated several times to verify

in glass tubes and placed in constant temperature to equilibrate. Samples

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			ORIGINAL MEASUREMENTS: Sunier, A.A.			
VARIABLES:			PREPARED	BY:		
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES		<u> </u>			
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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				
		AUXILIAR	(INFORMATIO	N		
METHOD: APPARATUS/PROCEDURE			SOURCE AND	D PURITY OF	MATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed			Compa	any, Rochesto ystallized so	fied, Eastman Kodak er, New York, USA, was everal times from meth-	
			anol.			

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Sunier, A.A.			
(2) Ethyl 2-furoate; C ₇ H ₈ O ₃ ; [614-99-3]			J. Phys. Chem. <u>1931</u> , 35, 1756-1761				
VARIABLES:			PREPARED	BY:			
Temperature	Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES				** **********************************		
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>×</i> 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					

increased. Solubility determined by visual noting the temperature at which the last ESTIMATED ERRORS:

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

T/K: precision \pm 0.1. x_1 : \pm 0.0002. (compiler).

SOURCE AND PURITY OF MATERIALS:

was used as received.

 Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from meth-

(2) Purity not given, Eastman Kodak Company,

(2) Purity not given, Eastman Kodak Company,

was used as received.

T/K: precision \pm 0.1. x_1 : \pm 0.0002. (compiler).

ESTIMATED ERRORS:

						12	
COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) n-Propyl 2-furoate; C ₈ H ₁₀ O ₃ ; [615-10-1] VARIABLES:			Sunier, A.A. J. Phys. Chem. <u>1931</u> , 35, 1756-1761.				
							PREPARED I
			Temperature	Temperature			ee, Jr.
EXPERIMENTAL	VALUES						
T/K	* ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	323.4 0.456 0.544						
		AUXILIARY	INFORMATION	·			
METHOD: APPAR	ATUS/PROCEDU	RE	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.			Company, Rochester, New York, USA, was recrystallized several times from meth anol. (2) Purity not given, Eastman Kodak Compan was used as received.				
						ıny,	
				eision ± 0.1.			

T/K: precision \pm 0.1. x_1 : \pm 0.0002. (compiler).

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Sunier, A.A.			
(2) n-Butyl 2-furoate; C ₉ H ₁₂ O ₃ ; [583-33-5]			J. Phys. Chem. <u>1931</u> , 35, 1756-1761.				
VARIABLES:	VARIABLES: Temperature			PREPARED BY:			
Temperature				W.E. Acree, Jr.			
EXPERIMENTAL	VALUES						
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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

results.

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:

- 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 \pm 0.1. x_1 : ± 0.0002. (compiler).

26				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Mahieu, J.			
(2) 1,1-Oxybisethane; C ₄ H ₁₀ O; [60-29-7]	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 0.753	0.247			
a computed by compiler from published so solubilities, which were expressed as we solute per 100 grams of solvent.				
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer,	(1) Purity and source not given.			
and a precision balance.	(2) Purity and source not given.			
Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solu-				
tions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained	ESTIMATED ERRORS:			
after solvent had evaporated.	T/K: precision + 0.5 (compiler).			

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

G.M.; Philip, W.G. D. Soc. <u>1928</u> , 1937-1942. DBY: Tree, Jr.		
BY:		
ree, Jr.		
0.3773		

METHOD: APPARATUS/PROCEDURE

after solvent had evaporated.

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 \pm 0.1. x_1 : 0.0001. (compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1-Ethoxypropane; C ₅ H ₁₂ O; [628-32-0]		ORIGINAL MEASUREMENTS:		
		Bennett, G.M.; Philip, W.G. J. Chem. Soc. 1928, 1937-1942.		
VARIABLES:				
Temperature				
EXPERIMENTAL VALUES				
T/K	<i>x</i> ₂	<i>x</i> ₁		
303.1	0.7292	0.2708		
312.9	0.6350	0.3650		
315.5	0.6064	0.3936		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.		(1) Purity and chemical source was not specified in paper.		
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		(2) Synthesized by authors, was purified by distillation.		
noting the temperature at which the last trace of solid solute disappeared. Meas- urements repeated several times to verify results.		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) 2-Ethoxypropane; C ₅ H ₁₂ O; [625-54-7] VARIABLES: Temperature		Bennett, G.M.; Philip, W.G. J. Chem. Soc. 1928, 1937-1942.		
		W.E. Acree, Jr.		
		EXPERIMENTAL VALUES		
T/K	<i>x</i> ₂	x_1		
317.1	0.5974	0.4026		
325.5	0.4864	0.5136		
	AUXILIARY	INFORMATION		
ETHOD: APPARATUS/PROC		INFORMATION SOURCE AND PURITY OF MATERIALS:		
ETHOD: APPARATUS/PROCE Constant temperature thermometer.	EDURE			
Constant temperature thermometer. Mixtures of known con in glass tubes and platemperature to equilified were rotated while bar	EDURE bath and a precision centrations sealed aced in constant brate. Samples th temperature slowly	SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source was not		
Constant temperature thermometer. Mixtures of known con in glass tubes and platemperature to equilibrium.	centrations sealed aced in constant brate. Samples th temperature slowly determined by visual e at which the last	SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source was not specified in paper. (2) Synthesized by authors, was purified		

120				
COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 2,2-Dimethyloxetane; C ₅ H ₁₀ O; [6245-99-4]		ORIGINAL MEASUREMENTS:		
		Bennett, G.M.; Philip, W.G. J. Chem. Soc. 1928, 1937-1942.		
				VARIABLES:
Temperature		W.E. Acree, Jr.		
EIPERIMENTAL VALUES				
T/K	x ₂	<i>x</i> ₁		
307.0	0.6990	0.3010		
313.1	0.5913	0.4087		
317.9	0.5443	0.4557		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.		(1) Purity and chemical source was not specified in paper.		
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		(2) Synthesized by authors, was purified by distillation.		
noting the temperature trace of solid solute	at which the last	ESTIMATED ERRORS:		
urements repeated severesults.		T/K : precision \pm 0.1. x_1 : 0.0001. (compiler).		

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 3,3-Dimethyloxetane; C ₅ H ₁₀ O; [6921-35-3]		ORIGINAL MEASUREMENTS:		
		Bennett, G.M.; Philip, W.G. J. Chem. Soc. 1928, 1937-1942.		
Temperature		W.E. Acree, Jr.		
EIPERIMENTAL VALUES				
T/K	x ₂	x ₁		
302.4	0.6540	0.3460		
312.1	0.5827	0.4173		
	AUXIL	IARY INFORMATION		
ETHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		

Constant temperature bath and a precision thermometer. $% \left(1\right) =\left(1\right) \left(1\right$

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 chemical source was not specified in paper.
- (2) Synthesized by authors, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : 0.0001. (compiler).

		123		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Tetrahydropyran; C ₅ H ₁₀ O; [142-68-7]		ORIGINAL MEASUREMENTS:		
		Bennett, G.M.; Philip, W.G.		
		J. Chem. Soc. <u>1928</u> , 1937-1942.		
VARIABLES:	IABLES: PREPARED BY:	PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	x ₂	<i>x</i> ₁		
299.6	0.6579	0.3421		
303.3	0.6295	0.3705		
313.4	0.5392	0.4608		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.		(1) Purity and chemical source was not specified in paper.		
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		(2) Synthesized by authors, was purified by distillation.		
increased. Solubility determined by visual inoting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.		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 ₂ Cl ₂ ; [75-09-2]		Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	x ₂	<i>x</i> ₁		
25.0 0.670		0.330		
	AUXILIARY	INFORMATION		
ETHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.		(1) Purity, source and purification procedures not specified.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		(2) Reagent Grade, J. T. Baker Chemical Company, USA, was used as received.		
noting the temperature	at which the last	ESTIMATED ERRORS:		
trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using $\ln x_1$ versus $1/T$ graph.		T/K: precision ± 0.1. x1: ± 2 % (relative error; compiler).		

130			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.		
(2) Trichloromethane; CHCl ₃ ; [67-66-3]	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	<i>x</i> ₁		
25.0 0.661	0.339		
AUXILIA	RY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.	Purity, source and purification procedures not specified.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visua			
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.	<pre>ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 2 % (relative error; compiler).</pre>		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Mahieu, J.
(2) Trichloromethane; CHCl ₃ ; [67-66-3]	Bull. Soc. Chim. Belgique 1936, 45, 667-677.
variables:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
PERFECTION	
EXPERIMENTAL VALUES	
. 190	

t/°C x₂* x₁* 25.0 0.660 0.340

 $^{\bf a}$ 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 \pm 0.5 (compiler). x_1 : \pm 5 % (relative error; compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Trichloromethane; CHCl ₃ ; [67-66-3]		ORIGINAL MEASUREMENTS:		
		Speyers, C.L. Am. J. Sci. 1902, 14, 293-302.		
				VARIABLES:
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		1		
T/K	x ₂	<i>x</i> 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/PROCE	DURE	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		(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.		
the residue was subjec		ESTIMATED ERRORS:		
decomposition.		T/K : precision \pm 0.1. x_1 : \pm 8 % (relative error, compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Heric, E.L.; Posey, C.D.		
(2) Tetrachloromethane; CCl ₄ ; [56-23-5]	J. Chem. Eng. Data <u>1964</u> , 9, 35-43.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EIPERIMENTAL VALUES	<u> </u>		
t/°C x ₂	x ₁		
25.0 0.7409	0.2591		
	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
·			
Constant temperature bath, thermometer, and a precision refractometer.	(1) Eastman Chemical Company, Rochester, New York, USA, was used as received.		
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	(2) Spectroquality, Matheson, Coleman and Bell, USA, was dried over phosphorous pentoxide and distilled to a final purity of 99.99 %.		
by making repetitive measurements after several additional days.	ESTIMATED ERRORS:		
	T/K: precision ± 0.01. x ₁ : precision ± 0.0005.		

COMPONENTS:

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Tetrachloromethane; CCl₄; [56-23-5]

EVALUATOR:

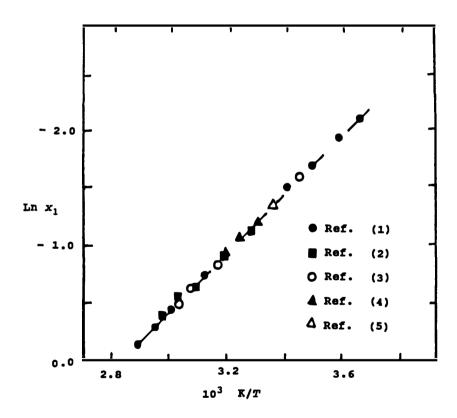
W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas August, 1994 76203-5068 (USA)

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:

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



Graphical plot of Ln x_1 versus 1/T

REFERENCES

- Ward, H.L. J. Phys. Chem. 1926, 30, 1316-1333.

 McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 2485-2488.

 Heric, E.L.; Yeh, K.-N. J. Chem. Eng. Data 1970, 15, 13-17.

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

 Heric, E.L.; Posey, C.D. J. Chem. Eng. Data 1964, 9, 35-43. 2. 3. 4.
- 5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Heric, E. L; Yeh, KN.			
(2) Tetrachloromethane; CCl ₄ ; [56-23-5]		J. Chem. Eng. Data <u>1970</u> , 15, 13-17.			
VARIABLES:			PREPARED BY:		
Temperature	Temperature		W.E. Acree, Jr.		
EIPERIMENTAL V	ALUES				
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	316.25 0.5671 0.4329		342.33	0.1935	0.8065
		AUXILIARY	INFORMATION	1	
METHOD: APPARA	METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.			nt Grade, Ba was used as	ker Chemical Company, received.	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		wass	tored over p	ker Chemical Company, hosphorous pentoxide rtly before use.	
noting the te	mperature at	which the last	ESTIMATED	ERRORS:	
trace of solid solute disappeared.		T/K: pred x ₁ : ± 0.0	ision <u>+</u> 0.03	•	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Chang, W.
(2) Tetrachloromethane; CCl ₄ ; [56-23-5]		Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EIPERIMENTAL VALUES		
t/°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 x₁ versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

- Purity, source and purification procedures not specified.
- (2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Tetrachloromethane; CC1 ₄ ; [56-23-5]			ORIGINAL I	ŒASUREMENTS	:		
			Ward, H.I	Ward, H.L.			
			J. Phys.	J. Phys. Chem. <u>1926</u> , 30, 1316-1333.			
VARIABLES:			PREPARED I	BY:			
Temperature			W.E. Acre	W.E. Acree, Jr.			
EXPERIMENTAL	VALUES						
T/K	x ₂	× ₁	T/K	<i>x</i> ₂	<i>x</i> 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 0.269	0.631 0.731		
292.7	0.783	0.217	338.0				
301.4	0.718	0.282	345.6	0.142	0.858		
		AUXIL	IARY INFORMATION	ī			
METHOD: APPAR	ATUS/PROCEDU	RE	SOURCE AND	PURITY OF	MATERIALS:		
Constant tem	Constant temperature bath and a precision				e not specified, was		

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.

- 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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

COMPONENTS:	COMPONENTS: (1) Naphthalene; C ₁₀ H; [91-20-3]			MEASUREMENTS:		
(1) Naphthal				McLaughlin, E.; Zainal, H.A. J. Chem. Soc. <u>1960</u> , 2485-2488.		
(2) Tetrachloromethane; CC1 ₄ ; [56-23-5]			J. Chem.			
VARIABLES:	VARIABLES:			BY:		
Temperature	Temperature			ee, Jr.		
EXPERIMENTAL	VALUES					
T/K	<i>x</i> ₂	<i>*</i> 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				
<u> </u>						

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:

- 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 \pm 0.1. x_1 : \pm 0.0003 (compiler).

						13	
COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Tetrachloromethane; CCl ₄ ; [56-23-5]			ORIGINAL P	ORIGINAL MEASUREMENTS:			
			C.L.	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.			
VARIABLES:			PREPARED E	PREPARED BY:			
T/K = 303, 308 and 313			W.E. Acre	W.E. Acree, Jr.			
EIPERIMENTAL '	VALUES		•				
t/° C	x ₂	<i>*</i> 1	t/° C	<i>x</i> ₂	<i>x</i> ₁		
30.0	0.6988	0.3012	40.0	0.6019	0.3981		
35.0 0.6538 0.3462							
		AUXILI	ARY INFORMATION	· · · · · · · · · · · · · · · · · · ·			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF P	IATERIALS:		
Constant temperature bath, calorimetric thermometer, and gas chromatograph.			(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrys lized 3 times from methanol.			1 -	
glass bottle for several Attainment o repetitive m	s and allowed days at const f equilibrium	Aliquots of sat	Chemi vania sieve	cal Company, , USA, was s	Fisher Scientific Pittsburgh, Penns tored over molecular led shortly before	ar	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Trichloroethylene; C ₂ HCl 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.

ESTIMATED ERRORS:

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

EXPERIMENTAL VALUES

chromatographically.

 $c_1/(\text{mol dm}^{-3})$ t/°C 23.0

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo-hexane. Concentrations determined

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 reversedphase 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: \pm 1. c_1 : \pm 5% (relative error; compiler).

COMPONENTS:			ORIGINAL M	easurements:		
 Naphthalene; C₈H₁₀; [91-20-3] Diiodomethane; CH₂I₂; [75-11-6] 			Domanska, U. Polish J. Chem. 1981, 55, 1715-1720. (numerical values obtained through personal communication with author.)			
VARIABLES:			PREPARED E	Y:		
Temperature			W.E. Acre	e, Jr.		
EXPERIMENTAL V	ALUES		ļ			
T/K	<i>x</i> ₂	<i>×</i> ₁	T/K	x ₂	<i>*</i> 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	1		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute dispressed.			(1) Purity not specified, P.O.Ch., Gliwice Poland, was vacuum sublimed to a melting temperature of 80.25 °C.			
					t specified, Chemapol, as received.	
			ESTIMATED	ERRORS:		

COMPONENTS:	COMPONENTS:			ORIGINAL MEASUREMENTS:		
 (1) Naphthalene; C₁₀H₈; [91-20-3] (2) 1,1-Dibromoethane; C₂H₄Br₂; [557-91-5] 		Sunier, A.A.; Rosenblum, C.				
		J. Phys. Chem. 1928, 32, 1047-1055.				
VARIABLES:			PREPARED BY:			
Temperature		W.E. Acre	ee, Jr.			
EXPERIMENTAL	VALUES		· · · · · · · · · · · · · · · · · · ·			
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x ₂	<i>*</i> 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				

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

trace of solid solute disappeared.

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 meth-
- (2) Purity not given, Eastman Kodak Company, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision \pm 0.1.

 x_1 : to 3 significant figs. (compiler).

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

	10			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.			
(2) 1,2-Dibromoethane; C ₂ H ₄ Br ₂ ; [106-93-4]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
Biperimental values				
t/°C x ₂	<i>x</i> ₁			
25.0 0.697	0.303			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	(1) Purity, source and purification procedures not specified.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) Reagent Grade, Eastman Organic Chem- ical, USA, was used as received.			
noting the temperature at which the last trace of solid solute disappeared. Sol-	ESTIMATED ERRORS:			
ubilities at 298 K interpolated from experimental values using ln x ₁ versus 1/T graph.	T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).			

COMPONENTS:	COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Naphthal			Sunier, A.A.; Rosenblum, C.				
(2) 1,2-Dibromoethane; C ₂ H ₄ Br ₂ ; [106-93-4]		J. Phys. Chem. <u>1928</u> , 32, 1047-1055.					
VARIABLES:			PREPARED	PREPARED BY:			
Temperature	Temperature		W.E. Acr	ee, Jr.			
EXPERIMENTAL '	VALUES		!				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	328.3 0.386 0.616						

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer. $% \left(\mathbf{r}_{i}\right) =\mathbf{r}_{i}$

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:

- 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 \pm 0.1. x_1 : \pm 0.002. (compiler).

130				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.			
(2) 1,1-Dichloroethane; C ₂ H ₄ Cl ₂ ; [75-34-3]	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	<i>x</i> ₁			
25.0 0.691	0.309			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	(1) Purity, source and purification procedures not specified.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.			
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.	<pre>ESTIMATED ERRORS: T/K: precision ± 0.1. x₁: ± 2 % (relative error; compiler).</pre>			

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1,1-Dichloroethane; C ₂ H ₄ Cl ₂ ; [75-34-3] VARIABLES: Temperature			ORIGINAL	ORIGINAL MEASUREMENTS: Sunier, A.A.; Rosenblum, C. J. Phys. Chem. 1928, 32, 1047-1055. PREPARED BY:			
			Sunier,				
			J. Phys.				
			PREPARED				
			W.E. Acr	W.E. Acree, Jr.			
EXPERIMENTAL	VALUES		!				
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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					
		AUXIL	IARY INFORMATION	4			
ŒTHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF	MATERIALS:		
Constant temperature bath and a precision thermometer.			Compa	ny, Rochestostallized so	fied, Eastman Kodak er, New York, USA, wa everal times from met		

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. Meas-

urements repeated several times to verify

results.

ESTIMATED ERRORS:

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

anol.
(2) Purity not given, Eastman Kodak Company,

was distilled shortly before use.

	139
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Chang, W.
(2) 1,2-Dichloroethane; C ₂ H ₄ Cl ₂ ; [107-06-2]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C × ₂	x ₁
25.0 0.680	0.320
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.	 Purity, source and purification procedures not specified.
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual	(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.
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.	ESTIMATED ERRORS: T/K : precision \pm 0.1. x_1 : \pm 2 % (relative error; compiler).

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		ORIGINAL MEASUREMENTS:				
		Sunier, A.A.; Rosenblum, C. J. Phys. Chem. <u>1928</u> , 32, 1047-1055.				
(2) 1,2-Dichloroethane; C ₂ H ₄ Cl ₂ ; [107-06-2]						
VARIABLES:	Temperature		PREPARED BY:			
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	x ₂	<i>x</i> 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		0.918	
324.3 0.428 0.572						

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

 $1/\bar{T}$ graph.

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 \pm 0.1. x_1 : \pm 0.002. (compiler).

140					
COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Chang, W.			
(2) Chlorobenzene; C ₆ H ₅	c1; [108-90-7]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).			
VARIABLES:		PREPARED BY:			
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES		4			
t/°C	<i>x</i> ₂	х 1			
25.0	0.689	0.311			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature by thermometer.	ath and a precision	(1) Purity, source and purification procedures not specified.			
Mixtures of known concin glass ampoules and ptemperature to equilibuter rotated while bath increased. Solubility	placed in constant rate. Samples n temperature slowly	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.			
noting the temperature trace of solid solute oublitties at 298 K into experimental values usi 1/T graph.	at which the last disappeared. Sol- erpolated from	ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 2 % (relative error; compiler).			

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Chlorobenzene; C ₆ H ₅ Cl; [108-90-7]		ORIGINAL MEASUREMENTS: Ward, H.L. J. Phys. Chem. 1926, 30, 1316-1333.									
						VARIABLES:			PREPARED	BY:	<u> </u>
						Temperature	Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VA	LUES		1								
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>*</i> 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							
	0.651	0.349									

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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

COMPONENTS:	_	ORIGINAL MEA	SUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈	; [91-20-3]	Morris, R.E.; Cook, W.A.				
(2) 1,4-Dichlorobenze [106-46-7]			J. Am. Chem. Soc. <u>1935</u> , 57, 2403-2406.			
VARIABLES:						
Temperature		W.E. Acree,	Jr.			
EIPERIMENTAL VALUES						
T/K	x ₂	<i>×</i> 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. $% \left(1\right) =\left(1\right) \left(1\right$

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:

- Purity and chemical source were not specified, was purified by distillalation.
- (2) Purity and chemical source were not specified, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.001.

		1				
COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		McLaughlin, E.; Messer, C.E.				
(2) Hexafluorobenzene;	C ₆ F ₆ ; [392-56-3]	J. Chem. Soc., Sect. A 1966, 1106-1110.				
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
T/K	<i>x</i> ₂	<i>x</i> 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/PROCED	URE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bathermometer. Mixtures of known conce	entrations sealed	(1) Molecular Weight Grade, Hopkin and Williams, was passed over an alumina column, recrystallized and sublimed.				
in glass ampoules and p temperature to equilibr were rotated while bath increased. Solubility of	ate. Samples temperature slowly	(2) Purity not given, Imperial Smelting, Ltd., Avonmouth, Bristol, was dried over anhydrous calcium sulfate.				
noting the temperature trace of solid solute d	at which the last	ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 0.0003 (compiler).				

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M.
(2) Octafluoronaphthalene; C ₁₀ F ₈ ; [313-72-4]	Bull. Chem. Soc. Japan <u>1985</u> , 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.

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. (2) Reagent grade, Tokyo Chemical Company, Japan, was recrystallized from methanol before use. ESTIMATED ERRORS: T/K: precision ± 0.3 (Compiler). x1: ± 0.02 (Compiler).

COMPONENTS:

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Methanol; CH,O; [67-56-1]

EVALUATOR:

W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-506 August, 1994 76203-5068 (USA)

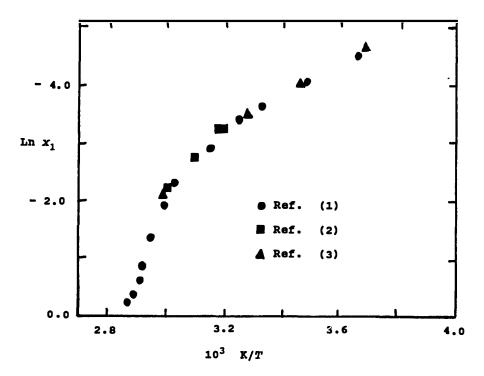
CRITICAL EVALUATION:

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:

$$\text{Ln } x_1 = -5574.0 \ (1/T) + 14.998 \ (r = 0.9280)$$

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

- Ward, H.L. J. Phys. Chem. 1926, 30, 1316-1333.
 Sunier, A.A. J. Phys. Chem. 1930, 34, 2582-2597.
 Speyers, C.L. Am. J. Sci. 1902, 14, 293-302.
 Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. J. Chem. Eng. Data 1989, 34, 438-443.
- Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, 24, 639-646. 5.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Ward, H.L. (2) Methanol; CH₄O; [67-56-1] J. Phys. Chem. 1926, 30, 1316-1333. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K \mathbf{x}_{2} ×1 274.0 0.989 0.0107 0.0163 286.7 0.984 0.974 0.0255 299.5 306.8 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).

OPICINAL MEASUREMENTS. COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Sunier, A.A. (2) Methanol; CH₂O; [67-56-1] J. Phys. Chem. 1930, 34, 2582-2597. PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EIPERIMENTAL VALUES T/K T/K *x*₁ X2 \mathbf{x}_2 x_1 0.6093 0.3907 341.8 313.4 0.9610 0.0390 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:

- 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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methanol; CH ₄ O; [67-56-1] VARIABLES: Temperature		ORIGINAL MEASUREMENTS:						
		Sunier, A.A. J. Phys. Chem. 1930, 34, 2582-2597. PREPARED BY:						
						W.E. Acree, Jr.		
						EXPERIMENTAL	VALUES	
		T/K	x ₂	<i>*</i> 1	T/K	x ₂	<i>x</i> 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 0.8	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:

- 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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

140					
COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methanol; CH ₄ O; [67-56-1]		Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. J. Chem. Eng. Data 1989, 34, 438-443.			
VARIABLES:		PREPARED BY:			
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES		•			
t/°C	* ₂	<i>x</i> ₁			
25.0	0.9765	0.0235			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature b and an ultraviolet spe		(1) Scintillation grade, 99 %, source not given.			
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 spectro-		(2) 99.9 %, source not given.			
photometric analysis a	t 254 nm.	ESTIMATED ERRORS:			
		T/K: precision \pm 0.05 (compiler). x_1 : \pm 5 % (relative error; compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methanol; CH ₄ O; [67-56-1]	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 0.6	16			
AUXILIARY	INFORMATION			
ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.			
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a 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	(2) Purity and chemical source not given, purification procedure not specified.			
fluorescence or uv detection.	ESTIMATED ERRORS:			
	T/K : \pm 1. c_1 : \pm 5% (relative error; compiler).			

					1		
COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Methanol; CH ₄ O; [67-56-1] VARIABLES:			ORIGINAL MEASUREMENTS: Speyers, C.L.				
							Ат. J. Sci. <u>1902</u> , 14, 293-302.
			PREPARED BY:				
			Temperature			W.E. Acree, Jr.	
EXPERIMENTAL	VALUES		_				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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					
		AUXILIAR	Y INFORMATION	N			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	iaterials:		
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		tall: point (2) Marke dried	ized from ald t temperature ed "Acetonfre	Kahlbaum, was recrystohol to a melting of 80.1 °C. i", from Kahlbaum, m oxide and distilled			
	cion co dryne		BCMTV1MBD	BDDODC.			

ESTIMATED ERRORS:

T/K: precision \pm 0.1.

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

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Ethanol; C ₂ H ₆ O; [64-17-5]			ORIGINAL	ORIGINAL MEASUREMENTS: Speyers, C.L.			
			Speyers,				
			Ат. J. Sci. <u>1902</u> , 14, 293-302.				
VARIABLES:			PREPARED 1	BY:		•	
Temperature	Temperature			W.E. Acree, Jr.			
EXPERIMENTAL '	VALUES		<u> </u>				
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x ₂	<i>×</i> 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					
			MARY INFORMATION				

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes.

minutes. Saturated solution was with-drawn through a coarse filter and anal-yzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

METHOD: APPARATUS/PROCEDURE

the residue was subject to too much

decomposition.

SOURCE AND PURITY OF MATERIALS:

- 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 \pm 0.1. x_1 : \pm 8 % (relative error, compiler).

COMPONENTS:

- (1) Naphthalene; C10H8; [91-20-3]
- (2) Ethanol; C₂H₆O; [64-17-5]

EVALUATOR:

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

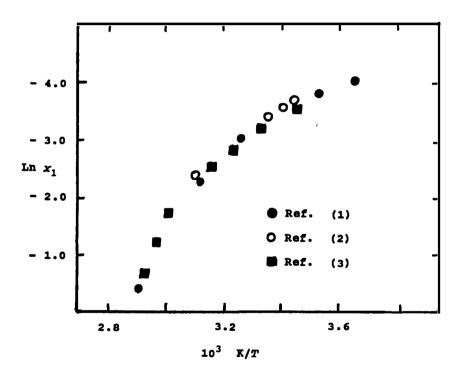
CRITICAL EVALUATION:

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 $\operatorname{Ln} x_1$ versus 1/T yielded the following mathematical relationship:

$$Ln x_1 = -4761.8 (1/T) + 12.740$$
 (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.
- Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. J. Chem. Eng. Data 1989, 34, 438-443.

					14	
COMPONENTS:		ORIGINAL M	ŒASUREMENTS	:		
(1) Naphthale	ene; C ₁₀ H ₈ ; [91-20-3]	Domanska, U.			
(2) Ethanol; C ₂ H ₆ O; [64-17-5] VARIABLES:			Polish J. Chem. 1981, 55, 1715-1720. (numerical values obtained through personal correspondence with author.)			
			PREPARED E	Y:		
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL V	ALUES					
T/K	x 2	<i>x</i> ₁	T/K	x ₂	* 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: APPARA	TUS/PROCEDU	RE	SOURCE AND	PURITY OF P	(ATERIALS:	
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		Gliwi to a (2) Initi Polan toxido	ce, Poland, melting temp al purity no d, was dried	fied, P.O.Ch., was vacuum sublimed perature of 80.25 °C. pt specified, Reachim., d over phosphorous pen- lonally distilled to a 19.9+ %.		
		olid disappeared.	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) Ethanol; C ₂ H ₆ O; [64-17-5]			ORIGINAL	ORIGINAL MEASUREMENTS: Sunier, A.A.		
			Sunier,			
			J. Phys.	J. Phys. Chem. <u>1930</u> , 34, 2582-2597.		
VARIABLES:			PREPARED BY:			
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	x 2	<i>x</i> 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. 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 \pm 0.1. x_1 : ± 0.0002. (compiler).

COMPONENTS:

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) Ethanol; C₂H₆O; [64-17-5]

VARIABLES:

T/K = 298

ORIGINAL MEASUREMENTS:

Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.

J. Chem. Eng. Data 1989, 34, 438-443.

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C

 x_2

25.0 0.9602

*x*₁

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:

- Scintillation grade, 99 %, source not given.
- (2) 200 Proof, source not given.

ESTIMATED ERRORS:

T/K: precision \pm 0.05 (compiler). x_1 : \pm 5 % (relative error; compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1-Propanol; C ₃ H ₈ O; [71-23-8] VARIABLES: Temperature			ORIGINAL N	ORIGINAL MEASUREMENTS: Sunier, A.A.				
			Sunier, A					
			J. Phys.	J. Phys. Chem. <u>1930</u> , 34, 2582-2597.				
			PREPARED BY: W.E. Acree, Jr.					
							EXPERIMENTAL	VALUES
T/K	<i>x</i> ₂	<i>x</i> 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:

- 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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

- (1) Naphthalene; $C_{10}H_8$; [91-20-3]
- (2) 1-Propanol; C₃H₈O; [71-23-8]

EVALUATOR:

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

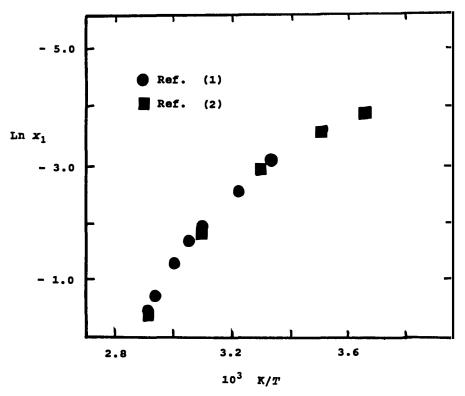
CRITICAL EVALUATION:

Naphthalene solubilities in 1-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:

$$\operatorname{Ln} x_1 = -4803.1 (1/T) + 13.193 \qquad (r = 0.9694)$$

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

- Sunier, A.A. J. Phys. Chem. <u>1930</u>, 34, 2582-2597.
- 2. Speyers, C.L. Am. J. Sci. 1902, 14, 293-302.
- Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. J. Chem. Eng. Data 1989, 34, 438-443.

102				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Dickhut, R.M.; Andren, A.W.; Armstrong, D.E.			
(2) 1-Propanol; C ₃ H ₈ O; [71-23-8]				
	J. Chem. Eng. Data 1989, 34, 438-443.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°c x ₂	<i>x</i> ₁			
25.0 0.9495	0.0505			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer, and an ultraviolet spectrophotometer.	(1) Scintillation grade, 99 %, source not given.			
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 spectro-	(2) 99.5 %, source not given.			
photometric analysis at 254 nm.	ESTIMATED ERRORS:			
	T/K: precision \pm 0.05 (compiler). x_1 : \pm 5 % (relative error; compiler).			

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1-Propanol; C ₃ H ₈ O; [71-23-8] VARIABLES: Temperature			ORIGINAL MEASUREMENTS: Speyers, C.L. Am. J. Sci. 1902, 14, 293-302.						
							PREPARED BY:		
							W.E. Acre	W.E. Acree, Jr.	
			EXPERIMENTAL V	ALUES		1			
			T/K	x 2	<i>x</i> ₁	T/K	x 2	<i>x</i> 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: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:				
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing			 (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. 						
that evaporat the residue w decomposition	as subject to		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]	Sunier, A.A.			
(2) 2-Propanol; C ₃ H ₈ O;	[67-63-0]	J. Phys. Chem. <u>1930</u> , 34, 2582-2597. PREPARED BY:		J. Phys. Chem. <u>1930</u> , 34, 2582-2597.	
VARIABLES:					
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	x ₂	<i>x</i> 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			

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:

- 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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3]

EVALUATOR:

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

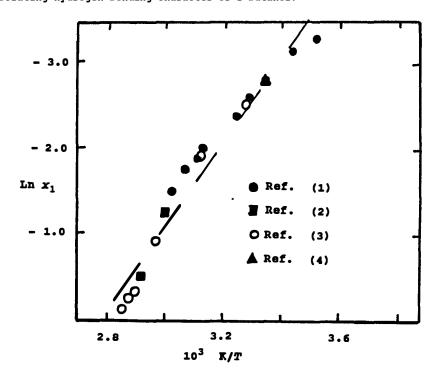
CRITICAL EVALUATION:

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:

$$\operatorname{Ln} x_1 = -4963.6 (1/T) + 13.865$$
 (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.
- Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. J. Chem. Eng. Data 1989, 34, 438-443.

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) 1-Butanol; C4H10O; [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	<i>x</i> 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:

- 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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) 1-Butanol; C4H10O; [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	<i>x</i> 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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

			ORIGINAL MEASUREMENTS:		
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Sunier, A.A.		
(2) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]		J. Phys. Chem. <u>1930</u> , 34, 2582-2597.			
VARIABLES:			PREPARED I	BY:	
Temperature	Temperature		W.E. Acre	ee, Jr.	
	VALUES		·		
EXPERIMENTAL					
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x 2	<i>*</i> ₁
	x ₂ 0.9061	* ₁ 0.0939	<i>T/</i> K 341.6	x ₂ 0.3745	* ₁ 0.6255
T/K	-	•	•	_	•

METHOD: APPARATUS/PROCEDURE

COMPONENTS:

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:

- 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:

ORIGINAL MEASUREMENTS:

T/K: precision \pm 0.1. x_1 : \pm 0.0002. (compiler).

		ONIONNE PEROONERENTO		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1-Butanol; C ₄ H 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	<i>x</i> 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 \pm 0.05 (compiler). x_1 : \pm 5 % (relative error; compiler).

100												
COMPONENTS:			ORIGINAL P	ŒASUR EJŒN TS:								
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6] VARIABLES:			Sunier, A.A. J. Phys. Chem. 1930, 34, 2582-2597. PREPARED BY:									
							Temperature	Temperature			e, Jr.	
							EXPERIMENTAL '	VALUES		!		
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>*</i> 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	INFORMATIO	N								
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:							
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			Comparecry anol.	any, Rocheste ystallized se . not given,	ied, Eastman Kodak ir, New York, USA, was veral times from meth- Eastman Kodak Company, irtly before use.							
noting the te	emperature at id solute dis	which the last appeared. Meas-	ESTIMATED	ERRORS:								
trace of solid solute disappeared. Measurements repeated several times to verify results.				cision \pm 0.1. 0002. (compile								

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Sunier, A.A.			
(2) 2-Methyl-1-propanol; C ₄ H ₁₀ O; [78-83-1]			J. Phys. Chem. <u>1930</u> , 34, 2582-2597.				
VARIABLES:			PREPARED BY:				
Temperature	Temperature		W.E. Acree, Jr.				
EXPERIMENTAL '	VALUES		<u>!</u>				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>*</i> 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					

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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

omponents:		ORIGINAL MEASUREMENTS:			
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Sunier, A.A.		
(2) 2-Methyl-2-propanol; C ₄ H ₁₀ O; [75-65-0]			J. Phys. Chem. <u>1930</u> , 34, 2582-2597.		
VARIABLES:			PREPARED I	BY:	
Temperature	Temperature		W.E. Acre	ee, Jr.	
EXPERIMENTAL	VALUES				
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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			

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:

- 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 \pm 0.1. x_1 : \pm 0.0002. (compiler).

MPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1-Pentanol; C ₅ H ₁₀ O; [71-41-0]		Dickhut, R.M.; Andren, A.W.; Armstrong, D.E. J. Chem. Eng. Data 1989, 34, 438-443.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
T/K = 298		w.L. Acree, JI.		
•		w.L. Acree, or.		
T/K = 298 EXPERIMENTAL VALUES t/°C	× ₂	w.E. Acree, 51.		

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:

- Scintillation grade, 99 %, source not given.
- (2) 99 %, source not given.

ESTIMATED ERRORS:

T/K: precision \pm 0.05 (compiler). x_1 : \pm 5 % (relative error; compiler).

160 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Domanska, U. Polish J. Chem., 1981, 55, 1715-1720. (numerical values obtained through (2) 1-Hexanol; C₆H₁₆O; [111-27-3] personal correspondence with author.) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K x₂ *x*₁ 282.30 0.946 0.054 286.35 0.936 0.062 0.073 0.927 290.35 296.05 0.914 0.086 299.95 0.899 0.101

0.880

0.853

0.825

0.799

0.776

0.632

AUXILIARY INFORMATION

0.120

0.147

0.175

0.201

0.224

0.368

METHOD: APPARATUS/PROCEDURE

305.75

310.85

314.95

318.95

321.45

331.55

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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Domanska, U. Polish J. Chem., 1981, 55, 1715-1720. (numerical values obtained through (2) 1-Octanol; C₈H₁₈O; [111-87-5] personal correspondence with author.) VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K $\mathbf{x_2}$ 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

AUXILIARY INFORMATION

0.328

0.422

METHOD: APPARATUS/PROCEDURE

325.95

331.55

Constant temperature bath and a precision thermometer.

0.672

0.578

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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

102				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. 1985, 19, 522-529.			
(2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]				
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EIPERIMENTAL VALUES	1			
t/°C	(mol dm ⁻³)			
25.0 0.9	589			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.	(1) Highest available commercial purity, specific chemical supplier not given, was used as received.			
Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 %	(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.			
SE30 ultraphase column.	ESTIMATED ERRORS:			
	T/K: ± 0.1 (compiler). c: ± 3 % (relative error; compiler).			

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Naphtha	lene; C ₁₀ H ₈ ; [91-20-3]	Weissenberger, G.			
(2) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0] VARIABLES: Temperature			Z. Angew Chem. 1927, 40, 776. PREPARED BY:			
			EXPERIMENTAL	VALUES		<u>!</u>
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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				
	*************************************	AUXILIA	RY INFORMATION			
METHOD: APPAR	RATUS/PROCEDU	RE	SOURCE AND PUR	TY OF MATERIA	ALS:	
Experimental paper.	details were	e not given in	(1) Purity and chemical source was not specified in paper.			
			(2) Purity and chemical source was not specified in paper.			
			ESTIMATED ERROR	RS:	T'	
			T/K: precision x ₁ : 0.002. (co	$n \pm 0.5$. (compospiler).	piler)	
,						

COMPONENTS:			ORIGINAL MEASU	ORIGINAL MEASUREMENTS:				
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Weissenberger	Weissenberger, G.				
(2) Methylc [25639-	yclohexanol; (42-3]	C ₇ H ₁₄ O;	Z. Angew Chem. <u>1927</u> , 40, 776.		Z. Angew Chem. <u>1927</u> , 40, 776.			
VARIABLES:			PREPARED BY:	EPARED BY:				
Temperature	mperature		W.E. Acree, J	r.				
EXPERIMENTAL	VALUES							
T/K	×2	<i>x</i> 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						
		AUXILIA	ARY INFORMATION					
METHOD: APPAI	RATUS/PROCEDUR	RE	SOURCE AND PURI	TY OF MATERIA	Ls:			
Experimental details were not given in paper.			(1) Purity and specified		irce was not			
			(2) Purity and specified		irce was not			
			ESTIMATED ERROF	RS:				
			T/K: precision x ₁ : 0.002. (co		oiler)			

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [99-65-0] (2) 1,4-Benzenediol; C ₆ H ₆ O ₂ ; [123-31-9] VARIABLES: Temperature			ORIGINAL MEASUREMENTS:			
			Kremann, R.; Janetzky, E.			
			Monatsch. Chem. <u>1911</u> , 32, 1055-1062.			
			PREPARED BY:			
			W.E. Acree, Jr	:•		
EXPERIME	ENTAL VALUES			,		
	T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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/PI	ROCEDURE		SOURCE AND PURI	TY OF MATERIA	ALS:
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,				(1) Purity and chemical source not give		
			(2) Purity and chemical source not given			
tempera	ture slowly	varied, and by visually	the phase	ESTIMATED ERROR	S:	
tempera	ture at which	ch the last/ Lsappeared/a	first	T/K : precision x_1 : \pm 0.002 (Co		iler).

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		ORIGINAL MEASUREMENTS:
		Kremann, R.; Janetzky, E.
(2) 1,2-Benzenediol;	C ₆ H ₆ O ₂ ; [120-80-9]	Monatsch. Chem. <u>1911</u> , 32, 1055-1062
VARIABLES:		PREPARED BY:
Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		-
T/K	* 2	× 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

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 \pm 0.2 (Compiler). x₁: \pm 0.002 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H	; [91-20-3]	Kremann, R.; Janetzky, E. Monatsch. Chem. <u>1911</u> , 32, 1055-1062.		
(2) 1,3-Benzenediol;	c ₆ H ₆ O ₂ ; [108-46-3]			
ARIABLES:		PREPARED BY:		
Temperature	Temperature		Jr.	
EIPERIMENTAL VALUES	***************************************			
T/K	x ₂	<i>x</i> 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 sys	tem.	

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:

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

ESTIMATED ERRORS:

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

166	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Sunier, A.A.
(2) Furfuryl Alcohol; C ₅ H ₆ O ₂ ; [98-00-0]	J. Phys. Chem. <u>1931</u> , 35, 1756-1761.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
<i>T/</i> K	<i>x</i> 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 METHOD: APPARATUS/PROCEDURE	INFORMATION 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. Meas-	(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from meth- anol. (2) Purity not given, Eastman Kodak Company was used as received. ESTIMATED ERRORS:
urements repeated several times to verify results.	T/K : precision \pm 0.1. x_1 : \pm 0.0002. (compiler).

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) 2-Propanone; C₃H₆O; [67-64-1]

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
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

METEOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer. $% \left(\mathbf{r}\right) =\left(\mathbf{r}\right)$

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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

100				
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Chang, W.		
(2) Carbon disulfide;	Carbon disulfide; CS ₂ ; [75-15-0] Ph.D Dissertation, North Dakota S versity, North Dakota, USA (1969)			
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	x ₂	× ₁		
25.0	0.717	0.283		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature between thermometer.	ath and a precision	(1) Purity, source and purification procedures not specified.		
Mixtures of known condin glass ampoules and temperature to equilibuser rotated while bat increased. Solubility	placed in constant rate. Samples h temperature slowly	(2) Reagent Grade or better, source not specified, was used as received.		
noting the temperature trace of solid solute ubilities at 298 K intexperimental values us 1/T graph.	at which the last disappeared. Sol- erpolated from	ESTIMATED ERRORS: T/K: precision ± 0.1. x ₁ : ± 2 % (relative error; compiler).		

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Mahieu, J.
(2) Carbon disulfide; CS ₂ ; [75-15-0]	Bull. Soc. Chim. Belgique 1936, 45, 667-677.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	!
t/°C ×2ª	x ₁ a
25.0 0.714	0.286
a computed by compiler from published so solubilities, which were expressed as we solute per 100 grams of solvent. AUXILIARY	eight percent and grams of INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant	(1) Purity and source not given.(2) Purity and source not given.
temperature. Aliquots of saturatured solu-	

ORIGINAL MEASUREMENTS:

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Ward, H.L.			
(2) Nitroben	(2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]			J. Phys. Chem. <u>1926</u> , 30, 1316-1333.		
VARIABLES:			PREPARED I	BY:		
Temperature			W.E. Acr	W.E. Acree, Jr.		
EXPERIMENTAL	VALUES		<u> </u>			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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				

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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

	ene: CH.: [9	COMPONENTS:			ORIGINAL MEASUREMENTS:			
(0) 11/1	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Srivastava, R.D.; Gupta, P.D.				
(2) Nitroben	zene; C ₆ H ₅ NO ₂	[98-95-3]	J. Indian Chem. Soc. <u>1967</u> , 44, 960					
Variables:			PREPARED	BY:				
Temperature			W.E. Acre	W.E. Acree, Jr.				
EXPERIMENTAL V	ALUES							
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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						
		AUXILI	ARY INFORMATION	ī				
ŒTHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:			
Constant temperature bath and a precision thermometer.				ed Kingdom, w	British Drug Houses as recrystallized and			

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

(2) Purity not given, British Drug Houses, was dried and distilled.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 3 % (relative error, Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]		Kremann, R. Monatsch. Chem. <u>1904</u> , 25, 1271-1292.		
		VARIABLES:		
Temperature		, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	W.E. Acree, Jr.	
EXPERIMENTAL VALUES				
T/K	x ₂	<i>x</i> 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)	
			0.137 and T/K = 267.2.	

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:

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

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Naphthal	(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Ward, H.L.			
(2) Aniline; C ₆ H ₇ N; [62-53-3]		J. Phys. Chem. <u>1926</u> , 30, 1316-1333.				
VARIABLES:	ARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL	VALUES				<u> </u>	
T/K	x ₂	* 1	T/K	x ₂	* 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	

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:

- 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 \pm 0.1. x_1 : to 3 significant figs. (compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Thiophene; C ₄ H ₄ S; [110-02-1]			ORIGINAL I	ORIGINAL MEASUREMENTS:				
			Choi, P.	Choi, P.B.; McLaughlin, E.				
			Ind. Eng	Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-51.				
VARIABLES:			PREPARED	BY:				
Temperature			W.E. Acree, Jr.					
EXPERIMENTAL	VALUES							
T/K	x 2	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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			
	0.4490	0.5510	348.1	0.0833	0.9167			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer. $% \left(1\right) =\left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left($

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 \pm 0.1. x_1 : \pm 0.0003.

172						
COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]			Choi, P.B.; McLaughlin, E.			
(2) Pyridine; C ₅ H ₅ N; [110-86-1] VARIABLES:			Ind. Eng. Chem. Fundam. 1983, 22, 46-51. PREPARED BY:			
EXPERIMENTAL V	VALUES		<u>.</u>			
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	× 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	333.2 0.3192 0.6808					
		AUXILIARY	INFORMATION	ı		
METHOD: APPAR	METHOD: APPARATUS/PROCEDURE			PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			Roche over talli (2) Gold Compa	ester, New Yo activated al .zed from tol .Label, 99.9+ .ny, was used	odiak Chemical Company, rk, USA, was passed umina and then recrysuene. %, Aldrich Chemical as received.	
increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.			T/K: prec x ₁ : ± 0.0	cision ± 0.1.		

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Shinomiya, C.					
(2) 2-Nitrobenzaldehyde; C ₇ H ₅ NO ₃ ; [552-89-6]		Nihon Kagakkai Shi. <u>1939</u> , 60, 170-182.					
VARIABLES:	/ARIABLES:		PREPARED BY:				
Temperature	Temperature		W.E. Acree, Jr.				
EXPERIMENTAL	VALUES		<u> </u>				
T/K	<i>x</i> ₂	×1	T/K	x ₂	<i>*</i> 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: APPA	ETHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:				
No experimental details given in paper. Compiler speculates that the transition temperatures were probably determined by			(1) Purity and specified		urce were not		
visually observing the temperature corresponding to the first crystal formation (or complete liquefication).		(2) Purity and chemical source were not specified in paper.					
			ESTIMATED ERRORS:				
			T/K : precision \pm 0.3 (Compiler). x_1 : \pm 0.002 (Compiler).				

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Shinomiya, C. (2) 3-Nitrobenzaldehyde; C₇H₅NO₃; [99-61-6] Nihon Kagakkai Shi. 1939, 60, 170-182. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EIPERIMENTAL VALUES Solid Phase T/K ×₁ ×2 330.2 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) 0.000 1.000 353.2 (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:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: Shinomiya, C. (1) Naphthalene; C10Hg; [91-20-3] Nihon Kagakkai Shi. 1939, 60, 170-182. (2) 4-Nitrobenzaldehyde; C₇H₅NO₃; [555-16-8] PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₁ $\boldsymbol{x_2}$ 0.000 1.000 378.2 (2) 372.7 0.851 0.149 (2) 0.273 367.2 0.727 (2) 0.413 358.7 0.587 (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) 0.208 0.792 342.2 (1) 342.2 0.185 0.815 (1) 348.7 0.090 0.910 (1) 0.030 0.970 352.2 (1) 353.7 0.010 0.990 (1) 0.000 1.000 353.2 (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 \pm 0.3 (Compiler). x_1 : \pm 0.002 (Compiler).

(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 1-Chloro-3-nitrobenzene; C ₇ H ₅ NO ₃ ; [121-73-3]		ORIGINAL MEASUREMENTS:				
		Shinomiya, C. Nihon Kagakkai Shi. <u>1939</u> , 60, 170-182.				
						VARIABLES:
Temperature						
EXPERIMENTAL VALUES						
T/K	*2	* 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:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.002 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Shinomiya, C. (2) 1-Chloro-4-nitrobenzene; C₇H₅NO₃; [100-00-5] Nihon Kagakkai Shi. 1939, 60, 170-182. VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES Solid Phase T/K x₁ x_2 0.000 1.000 (2) 356.7 0.173 347.2 0.827 (2) 0.331 (2) 332.2 0.669 0.341 (2) 334.2 0.659 0.363 329.2 0.637 (2) 0.601 0.399 326.2 (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) 0.375 0.625 326.2 (1) 329.2 0.352 0.648 (1) 0.346 0.654 330.2 (1) 0.328 0.672 331.2 (1) 0.230 0.770 342.2 (1) 346.2 0.821 0.179 (1) 353.2 0.000 1.000 (1) Phase diagram depicted in paper shows a simple eutectic system. **AUXILIARY INFORMATION** SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE No experimental details given in paper. (1) Purity and chemical source were not Compiler speculates that the transition specified in paper. temperatures were probably determined by visually observing the temperature corresponding to the first crystal forma-(2) Purity and chemical source were not tion (or complete liquefication). specified in paper. ESTIMATED ERRORS: T/K: precision \pm 0.7 (Compiler).

 x_1 : ± 0.002 (Compiler).

COMPONENTS: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 2,4-Dinitroaniline; C ₆ H ₅ N ₃ O ₄ ; [97-02-9]		ORIGINAL MEASUREMENTS: Shinomiya, C. Nihon Kagakkai Shi. 1938, 59, 922-926.							
					VARIABLES:		PREPARED BY: W.E. Acree, Jr.		
					Temperature				
EIPERIMENTAL 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 i	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 \pm 0.3 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Shinomiya, C. (2) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] Nihon Kagakkai Shi. 1938, 59, 922-926. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase x₁ x, 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 1:1 Compound 0.914 397.2 0.038 1:1 Compound 0.962 353.2 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

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:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Hammick, D.L.; Hellicar, A. J. Chem. Soc. 1938, 761-763. (2) 1,3,5-Trimethyl-2,4,6-trinitrobenzene; C9H9N3O6; [602-96-0] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES x₂ Solid Phase T/K $\boldsymbol{x_1}$ 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) 0.63 0.37 478.4 (2) 465.7 0.51 0.49 (2) 450.2 0.40 0.60 (2) 433.2 0.29 0.71 (2) 0.80 408.7 0.20 (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:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.005 (Compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Kofler, A. Z. Physik. Chem., Pt. A. 1940, 187, 201-(2) 4-Nitro-1-methylbenzene; $C_7H_7NO_2$; [99-99-0] 210. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x_2 X₁ 1.00 0.00 (2) 325.2 0.89 0.11 (2) 320.2 0.21 314.2 0.79 (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) 0.62 328.2 0.38 (1) 335.2 0.29 0.71 (1) 0.81 343.2 0.19 (1) 0.09 0.91 349.2 (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

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.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.01 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Kremann, R.
(2) 4-Nitro-1-methylbenzene; C ₇ H ₇ NO ₂ ; [99-99-0]	Monatsch. Chem. <u>1904</u> , 25, 1271-1292.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.

IPERIMENTAL VALUES					
T/K	x ₂	×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

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:

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

ESTIMATED ERRORS:

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

ORIGINAL MEASUREMENTS: COMPONENTS: Sekiguchi, K.; Suzuki, E.; Tsuda, Y.; (1) Naphthalene; C₁₀H₈; [91-20-3] Shirotani, K.-I.; Okamoto, K. (2) 1,3-Dinitrobenzene; C₆H₄N₂O₄; [99-65-0] Chem. Pharm. Bull. 1984, 32, 658-664. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K $\boldsymbol{x_1}$ $\boldsymbol{x_2}$ 0.000 1.000 (2) 363.8 0.123 356.4 0.877 (2) 348.3 0.757 0.243 (2) 0.690 0.310 (2) 341.8 337.7 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 0.503 325.0 0.497 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) 0.351 0.649 328.9 (1) 330.7 0.328 0.662 (1) 0.301 0.699 332.7 (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:

- 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 \pm 0.5 (Compiler). x₁: \pm 0.002 (Compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Kremann, R. Monatsch. Chem. 1904, 25, 1271-1292. (2) 1,3-Dinitrobenzene; C6H6N2O6; [99-65-0] VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K T/K ×1 x₂ x_1 x₂ 0.089 360.7 1.000 0.000 348.2 0.911 356.2 0.939 0.061 351.7 0.032 0.968 352.2 0.875 0.125 353.8 0.000 1.000 348.2 0.789 0.211 Phase diagram suggests formation of a 1:1 naphthalene - 1,3-dinitro-339.7 0.720 0.280 benzene molecular compound having 333.2 0.661 0.339 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 = 323.6326.2 0.599 0.401 323.7 0.577 0.423 323.7. 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 0.381 324.9 0.619 328.7 0.353 0.647 329.5 0.340 0.660 0.276 334.5 0.724 0.243 337.4 0.757 0.205 0.795 340.7 345.7 0.121 0.879

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:

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

ESTIMATED ERRORS:

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

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] Kremann, R. Monatsch. Chem. 1904, 25, 1271-1292. (2) 1,3,5-Trinitrobenzene; C₆H₃N₃O₆; [99-35-4] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₁ x, 0.000 395.2 1.000 (2) 393.2 0.971 0.029 (2) 0.085 389.2 0.915 (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 0.564 1:1 Compound 424.0 0.436 423.7 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 0.318 0.682 1:1 Compound 418.2 414.2 0.287 0.713 1:1 Compound 409.7 0.246 0.754 1:1 Compound 0.803 1:1 Compound 402.2 0.197 0.148 0.852 1:1 Compound 391.2 381.2 0.127 0.873 1:1 Compound 363.2 0.077 0.923 1:1 Compound 0.051 351.2 0.949 Eutectic 0.029 0.971 352.7 (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 SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not specified in paper.

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.

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

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) 2-Nitrophenol; C ₆ H ₅ NO ₃ ; [88-75-5] VARIABLES:		Kremann, R.			
					Monatsch. Chem. 1904, 25, 1271-1292. PREPARED BY:
		Temperature	Temperature		
		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)		

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:

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

ESTIMATED ERRORS:

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

COMPONENTS: ORIGINAL MEASUREMENTS: Kremann, R. (1) Naphthalene; C₁₀H₈; [91-20-3] (2) 4-Nitrophenol; $C_6H_5NO_3$; [100-02-7] Monatsch. Chem. 1904, 25, 1271-1292. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase X1 x₂ 0.000 386.2 1.000 (2) 380.2 0.900 0.100 (2) 375.2 0.799 0.201 (2) 0.686 0.314 368.2 (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) 0.619 354.2 0.381 (2) 0.269 0.731 348.2 (2) 348.2 0.181 0.819 (1) 0.063 0.937 351.2 (1) 0.000 1.000 353.7 (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:

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

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL M	easurements:		
(1) Naphthalene; C ₁₀ H ₈	 (1) Naphthalene; C₁₀H₈; [91-20-3] (2) 2,4-Dinitro-1-methylbenzene; C₇H₆N₂O₄; [121-14-2] 		Kofler, A. Z. Physik. Chem., Pt. A. 1940, 187, 201-210.		
VARIABLES:		PREPARED BY	Y:		
Temperature		W.E. Acre	e, Jr.		
EXPERIMENTAL VALUES					
T/K	* 2	× 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

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.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.01 (Compiler).

188 COMPONENTS: ORIGINAL MEASUREMENTS: Kremann, R. (1) Naphthalene; C₁₀H₈; [91-20-3] Monatsch. Chem. 1904, 25, 1271-1292. (2) 2,4-Dinitro-1-methylbenzene; C₇H₆N₂O₄; [121-14-2] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES

NTAL 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C,0Hg; [91-20-3] Kremann, R. Monatsch. Chem. 1904, 25, 1271-1292. (2) 2,4-Dinitrophenol; C₆H₆N₂O₅; [51-28-5] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase $\boldsymbol{x_1}$ x, 383.2 1.000 0.000 (2) 377.2 0.888 0.112 (2) 0.771 (2) 369.2 0.229 0.676 0.324 (2) 363.2 362.7 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 0.469 1:1 Compound 365.2 0.531 365.2 0.509 0.491 1:1 Compound 0.497 1:1 Compound 365.2 0.503 0.458 0.542 365.2 1:1 Compound 1;1 Compound 365.2 0.447 0.553 364.7 0.423 0.577 1;1 Compound 0.629 363.7 0.371 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) 0.069 0.931 349.7 (1) 352.2 0.030 0.970 (1) 0.000 353.7 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:

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

ESTIMATED ERRORS:

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

ORIGINAL MEASUREMENTS: COMPONENTS: Nigam, R.K.; Dhillon, M.S. (1) Naphthalene; C₁₀H₈; [91-20-3] (2) 2,4,6-Trinitrophenol; $C_6H_3N_3O_7$; [88-89-1] Indian J. Chem. 1970, 8, 821-825. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase x, x_1 1.0000 0.0000 395.2 (2) 387.2 0.9135 0.0865 1:1 Compound 404.0 0.8246 0.1754 1:1 Compound 1:1 Compound 409.2 0.7855 0.2145 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

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).

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.0001 (Compiler).

COMPONENTS:		ORIGINAL MEA	SUREMENTS:	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Isoquinoline; C ₉ H ₇ N; [119-65-3]		Kravchenko, V.M.; Pastukhova, I.S. J. Appl. Chem. U.S.S.R. 1952, 25, 343-350. (English translation)		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES ^a				
T _{in} /K	$T_{\sf fin}/K$	x ₂	<i>x</i> 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. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ 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:

- 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

192	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Simons, J.H.; Linevsky, M.J.
(2) Perfluoro-dibutyl ether; C ₈ F ₁₈ O [308-48-5]	J. Am. Chem. Soc. 1952, 74, 4750-4751.
VARIABLES:	PREPARED BY:
T/K = 298 and 308	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C × ₂	× ₁
25.0 0.9974	0.00257
35.0 0.9960	0.00402
AUXII	LIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precisithermometer.	ion (1) Purity and source not given, was recrystallized two times from ethanol.
Mixtures of known concentrations placed in special solubility flask and equili- brated in a constant temperature bath if 48 hours. The entire saturated solution was withdrawn by suction. Solubility	fied, was synthesized by authors and distilled shortly before use.
based upon weight of undissolved solid, which remained in the solubility flask after solution was removed.	<pre>T/K: precision ± 0.5 (compiler). x₁: ± 3 % (relative error; compiler).</pre>

T		1
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ;	[91-20-3]	Simons, J.H.; Linevsky, M.J.
(2) Perfluoro-tripropylamine; C ₉ F ₂₁ N [338-83-0]		J. Am. Chem. Soc. <u>1952</u> , 74, 4750-4751.
VARIABLES:		PREPARED BY:
T/K = 298 and 308		W.E. Acree, Jr.
EXPERIMENTAL VALUES		· ·
t/°C	x ₂	<i>x</i> ₁
25.0	0.9970	0.00300
35.0	0.9954	0.00461
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCED	JRE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer.		(1) Purity and source not given, was recrystallized two times from ethanol.

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.

ESTIMATED ERRORS:

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

(2) Purity and specific isomer not specified, was synthesized by authors and distilled shortly before use.

COMPONENTS:			ORIGINAL MEASUREME	NTS:	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Benzene; C ₆ H ₆ ; [71-43-2]		Kravchenko, V.M.			
		Zhur. Fiz. Khim. 1939, 13, 133-145.			
(3) Methylbe			Zhui. Fiz. Khim.	1939, 1	.5, 155-145.
(3) Methylbe	nzene, c ₇ n ₈ ;	[100-00-3]			
VARIABLES:	··		PREPARED BY:		
Temperature,	Solvent comp	position	W.E. Acree, Jr.		
EXPERIMENTAL	VALUES				
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	* 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
		(Co:	ntinued on next page)	
		AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY	OF MATER	IALS:	
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 ch specified in before use.			
,			(3) Purity and ch specified in before use.		

ESTIMATED ERRORS:

T/K: precision \pm 0.2 (Compiler). x_2 : \pm 0.002 (Compiler). x_1 : \pm 0.002 (Compiler).

ALMANMITT .			antature impare	M 20.	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Benzene; C ₆ H ₆ ; [71-43-2]		ORIGINAL MEASUREM			
		Kravchenko, V.M.			
		Zhur. Fiz. Khim.	1939, 13	, 133-145.	
(3) Methylben) Methylbenzene; C ₇ H ₈ ; [108-88-3]				
ARIABLES:			PREPARED BY:		
Cemperature,	Solvent com	position	W.E. Acree, Jr.		
PERIMENTAL V	ALUES (Cont	inuation)			
T/K	x ₂	<i>×</i> ₁	T/K	* 2	<i>×</i> ₁
230.1	0.425	0.034	283.4	0.092	0.208
230.0	0.421	0.043	172.7	0.149	0.015
235.2	0.417	0.052	170.2	0.128	0.014
248.2	0.411	0.066	187.6	0.126	0.023
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			
	0.104				
	0.098	0.150			

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Naphthalene; C10Hg; [91-20-3] Kravchenko, V.M. (2) Benzene; C,H,; [71-43-2] Zhur. Fiz. Khim. 1939, 13, 989-1000. (3) 1,3-Dimethylbenzene; C₈H₁₀; [108-38-3] VARIABLES: PREPARED BY: Temperature, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES T/K T/K ×1 $\boldsymbol{x_2}$ 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 0.089 268.3 0.729 0.136 253.0 0.433 0.740 0.447 265.4 0.124 239.2 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 0.800 0.053 0.630 266.2 327.2 0.102 338.7 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 0.409 0.087 0.273 0.016 251.2 213.0 251.9 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 0.110 0.768 339.2 253.2 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

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

212.3

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.

0.273

0.023

SOURCE AND PURITY OF MATERIALS:

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

0.275

0.032

- (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:

220.3

T/K: precision \pm 0.2 (Compiler). x_2 : ± 0.002 (Compiler). x_1 : ± 0.002 (Compiler).

COMPONENTS:		ORIGINAL MEASUR	EMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Kravchenko, V.M.; Pastukhova, I.S.				
(2) Benzene;	C ₆ H ₆ ; [71-43	-2 <u>]</u>	Zhur. Fiz. Khi	m. <u>1953</u> , 27	, 822-834.	
(3) Isoquino	line; C ₉ H ₇ N;	[119-65-3]				
VARIABLES:			PREPARED BY:			
Temperature,	Solvent comp	position	W.E. Acree, Jr.	•		
EXPERIMENTAL V	ALUES					
T/K	x 2	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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:

- 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 \pm 0.2 (Compiler). x_2 : \pm 0.002 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS:

- (1) Naphthalene; C10H8; [91-20-3]
- (2) Acetonitrile; C₂H₃N; [75-05-8]
- (3) Water; H₂O; [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 x 10 ⁻⁴
0.0096	2.55×10^{-4}
0.0228	3.49×10^{-4}
0.0330	4.66×10^{-4}
0.0469	6.45 x 10 ⁻⁴
0.0594	10.23×10^{-4}
0.0733	14.17 x 10 ⁻⁴
0.0887	22.44 x 10 ⁻⁴
0.1125	50.23 x 10 ⁻⁴
0.1316	71.64 x 10 ⁻⁴
0.1898	27.45 x 10 ⁻³
0.2280	51.16 x 10 ⁻³

 $[^]a$ $x_2^{\,(s)}\colon$ initial mole fraction of binary solvent mixture; $c_1\colon$ 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 volume-tric 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: \pm 0.05. $x_2^{(s)}$: \pm 0.0001 (compiler). c_1 : \pm 5 % (relative error; compiler).

COMPONENTS:

- (1) Naphthalene; C10Hg; [91-20-3]
- (2) Methanol; CH₄O; [67-56-1]
- (3) Water; H₂O; [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 x 10 ⁻⁴
0.0294	2.68 x 10 ⁻⁴
0.0294	2.61 x 10 ⁻⁴
0.0432	2.94 x 10 ⁻⁴
0.0432	3.14 x 10 ⁻⁴
0.0579	3.54 x 10 ⁻⁴
0.0900	5.02×10^{-4}
0.1236	7.45 x 10 ⁻⁴
0.1936	18.47×10^{-4}
0.2732	50.31 x 10 ⁻⁴
0.3591	13.43×10^{-3}
0.4588	33.22 x 10 ⁻³

 $[^]a$ $x_2^{\,(s)}\colon$ initial mole fraction of binary solvent mixture; $c_1\colon$ 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 volume-tric 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:

- 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:

 $T/K: \pm 0.05.$ $x_2^{(8)}: \pm 0.0001$ (compiler). $c_1: \pm 5$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Sarker, M.; Wilson, D.
(2) 1-Propanol; C ₃ H ₈ O; [71-23-8]	J. Tennessee Acad. Sci. <u>1986</u> , 61, 69-74.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = Ambient Room Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, c₁/(mg L⁻¹), expressed in terms of the equation: $c_1/(mg L^{-1}) = 36.5 (1 + 3.8 \times 10^5 x_2^{3.86})$ 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 : \pm 0.001 (Compiler). x_1 : \pm 8 % (Relative error; Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Sarker, M.; Wilson, D.
(2) 1-Hexanol; C ₆ H ₁₄ O; [111-27-3]	J. Tennessee Acad. Sci. <u>1986</u> , 61, 69-74.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = Ambient Room Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, c₁/(mg L⁻¹), expressed in terms of the equation: $c_1/(mg L^{-1}) = 36.5 (1 + 2.0 \times 10^{10} x_2^{-3.16})$ 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 : \pm 0.0001 (Compiler).

 x_1 : \pm 8 % (Relative error; Compiler).

ORIGINAL MEASUREMENTS:
Sarker, M.; Wilson, D.
J. Tennessee Acad. Sci. <u>1986</u> , 61, 69-74.
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: $c_1/(mg\ L^{-1}) = 36.5\ (1 + 6.7 \times 10^3 \times_2^{2.53})$ Mole fraction compositions of 2-propanone ranged between $x_2 = 0.01$ to $x_2 = 0.10$

Mole fraction compositions of 2-propanone ranged between $x_2 = 0.01$ to $x_2 = 0.10$. **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Gas chromatographic equipped with flame (1) Purity and chemical source not given ionization detection. in paper. Binary mixtures were prepared by weight. Excess solute and solvent placed in closed glass bottles and allowed to equilbrate at (2) Purity and chemical source not given. (3) Purity and chemical source not given. ambient room temperature for several days. A 100 mL aliquot removed and naphthalene concentrated by hexane extraction. Con-ESTIMATED ERRORS: centrations determined by gas chromatography. T/K: Unknown.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Sarker, M.; Wilson, D.
(2) 2-Butanone; C ₄ H ₈ O; [78-93-3]	J. Tennessee Acad. Sci. <u>1986</u> , 61, 69-74.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = Ambient Room Temperature	W.E. Acree, Jr.
	j

EXPERIMENTAL VALUES

Actual experimental data not given in cited paper. Solubilities, $c_1/(mg\ L^{-1})$, expressed in terms of the equation: $c_1/(mg\ L^{-1}) = 36.5\ (1 + 3.4 \times 10^4\ x_2^{2.45})$ 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:

 x_2 : \pm 0.01 (Compiler).

 x_1 : \pm 8 % (Relative error; Compiler).

- 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 : \pm 0.01 (Compiler). x_1 : \pm 8 % (Relative error; Compiler).

COMPONENTS:

- (1) Naphthalene; C₁₀H₈; [91-20-3]
- (2) 1,2-Ethanediol; C₂H₆O₂; [107-21-1]
- (3) Water; H₂O; [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 VALUES⁸ t = 25.0 °C

*2 ^(s)	c ₁ /(mol dm ⁻³)	x2 ^(s)	c ₁ /(mol dm ⁻³)
0.0000	2.01 x 10 ⁻⁴	0.4300	94.95 x 10 ⁻⁴
0.0084	2.16 x 10 ⁻⁴	0.5640	20.19 x 10 ⁻³
0.0167	2.38 x 10 ⁻⁴	0.5867	23.98 x 10 ⁻³
0.0257	2.61 x 10 ⁻⁴	1.0000	85.04 x 10 ⁻³
0.0347	2.91 x 10 ⁻⁴		
0.0444	3.24×10^{-4}		
0.0540	3.50×10^{-4}		
0.0748	4.28 x 10 ⁻⁴		
0.0973	5.38 x 10 ⁻⁴		
0.1217	7.12 x 10 ⁻⁴		
0.1483	9.25 x 10 ⁻⁴		
0.1773	12.47×10^{-4}		
0.2443	23.67 x 10 ⁻⁴		
0.3266	47.53 x 10 ⁻⁴		

 $^{^{\}rm a}$ $x_2^{\rm (s)};$ initial mole fraction of binary solvent mixture; c₁: 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 volume-tric 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:

- 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:

 $T/K: \pm 0.05.$ $x_2^{(8)}: \pm 0.0001$ (compiler). $c_1: \pm 5$ % (relative error; compiler).

COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] (2) Ethyl ethanoate; C₄H₈O₂; [141-78-6] (3) Water; H₂O; [7732-18-5] VARIABLES: T/K = Ambient Room Temperature ORIGINAL MEASUREMENTS: Sarker, M.; Wilson, D. J. Tennessee Acad. Sci. 1986, 61, 69-74. 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	SOURCE AND PURITY OF MATERIALS:
Gas chromatographic equipped with flame ionization detection.	(1) Purity and chemical source not given in paper.
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	(2) Purity and chemical source not given. (3) Purity and chemical source not given.
concentrated by hexane extraction. Concentrations determined by gas chromatography.	T/K: Unknown. x ₂ : ± 0.001 (Compiler). x ₄ : ± 8 % (Relative error; Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Sarker, M.; Wilson, D.
(2) Pyridine; C ₅ H ₅ N; [110-86-1]	J. Tennessee Acad. Sci. 1986, 61, 69-74.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = Ambient Room Temperature	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: $c_1/(\text{mg L}^{-1}) = 36.5 \ (1 + 3.5 \times 10^4 \times_2^{2.60})$ 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:

- 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 : \pm 0.01 (Compiler). x_1 : \pm 8 % (Relative error; Compiler).

PERYLENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

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

benzene

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

1-octanol

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

204			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Perylene; C ₂₀ H ₁₂ ; [198-55-0]	Lissi, E.A.; Abuin, E.B.		
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. 1981, 26, 19-34.		
VARIABLES:	PREPARED BY:		
T/K = 293	W.E. Acree, Jr.		
EIPERIMENTAL VALUES			
t/°C	(mol dm ⁻³)		
20.0 0.00037			
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.		
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured fluorescence emission intensity.	(2) Purity and chemical source not given, purification procedure not specified.		
	ESTIMATED ERRORS:		
	T/K : ± 2 . c_1 : unknown.		

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Perylene; C ₂₀ H ₁₂ ; [1	.98-55-0]	Mishra, D.S.; Yalkowsky, S.H.
(2) Benzene; C ₆ H ₆ ; [71-	43-2]	Ind. Eng. Chem. Res., <u>1990</u> , 29, 2278-2283.
VARIABLES:		PREPARED BY:
T/K = 296		W.E. Acree, Jr.
EIPERIMENTAL VALUES		
t/°C	x ₂	<i>x</i> ₁
23.0	0.9604	0.0396
	AUIILIARY	(INFORMATION
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bathermometer, and an uv/photometer.		(1) Reagent grade, source not specified, was used as received.
Excess solute and solve screw-capped test tube equilibrate for 3 days tion in a constant temp Samples centrifuged for concentrations were det photometrically. Attai brium verified by repet	and allowed to with gentle agita- erature bath. 30 minutes and ermined spectro- nment of equili-	(2) Reagent grade, source not specified, was used as received.
4 days later.		ESTIMATED ERRORS:
		T/K: ± 0.1 (compiler). x: ± 5 % (relative error; compiler).

COMPONENTS: (1) Perylene; C₂₀H₁₂; [198-55-0] Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D. (2) 1-Octanol; C₈H₁₈O; [111-87-5] Environ. Sci. Technol. 1985, 19, 522-529. VARIABLES: PREPARED BY: T/K = 298 W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/ºC

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

25.0

0.003044

AUXILIARY INFORMATION

METBOD: 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:

- 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

 ${\tt 1,8-dihydroperfluorooctane}$

octafluoronaphthalene

G. Alcohols

ethanol

1-octanol

H. <u>Ketones</u>

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

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

200					
COMPONENTS: (1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		ORIGINAL	MEASUREMENTS:	B	
		Doane, E.P.; Drickamer, H.G.			
(2) n-Hexane	n-Hexane; C ₆ H ₁₄ ; [110-54-3]		J. Phys. Chem. 1955, 59, 454-457.		
VARIABLES:			PREPARED BY:		
T/K = 298, P	ressure		W.E. Acree, Jr.		
EXPERIMENTAL	VALUES				
P/atm	x ₂	<i>x</i> ₁	P/atm	* 2	× 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			
		AUXILIAR	INFORMATIO	4	
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
balance and l	Constant temperature bath, analytical balance and high pressure equipment.		Compa		tman Kodak Chemical er, New York, USA, was
Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount of saturated solution removed,		dried		ips Petroleum, was orous pentoxide and	
		ness, and con- eight of solid	ESTIMATED	ERRORS:	
residue.	tration determined from weight of solid		$x_1: \pm 1-3$	cision ± 0.1. % at atmosp % at the hig	heric pressure, and her pressures.

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		Lissi, E.A.; Abuin, E.B.		
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]		Bol. Soc. Chil. Quim. 1981, 26, 19-34.		
VARIABLES:		PREPARED BY:		
T/K = 293	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C	c ₁ /(mc	ol dm ⁻³)		
20.0	0.0270			
AU	XILIARY IN	FORMATION		

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:

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: \pm 2. c_1 : unknown.

COMPONENTS	OMPONENTS: (1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		ORIGINAL MEA	SUREMENTS	1
(1) Phenanth			Doane, E.P.; Drickamer, H.G.		
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]			J. Phys. Ch	J. Phys. Chem. <u>1955</u> , 59, 454-457.	
VARIABLES:			PREPARED BY:		
T/K = 298, P	essure		W.E. Acree,	Jr.	
EXPERIMENTAL V	/ALUES				
P/atm	<i>x</i> ₂	<i>*</i> 1	P/atm	<i>x</i> 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
	0.9728	0.0272	7000	0.9948	0.0052

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 con-tration determined from weight of solid residue.

- (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 \pm 0.1. x_1 : \pm 1-3 % at atmospheric pressure, and \pm 10 % at the higher pressures.

COMPONENTS:	omponents:			ORIGINAL MEASUREMENTS:			
(1) Phenanth	rene; C ₁₄ H ₁₀ ;	[85-01-8]	Doane, E.	P.; Drickame	er, H.G.		
(2) n-Octane	; c ₈ H ₁₈ ; [111-	65-9]	J. Phys.	J. Phys. Chem. <u>1955</u> , 59, 454-457.			
VARIABLES:			PREPARED I	PREPARED BY:			
T/K = 298, P	T/K = 298, Pressure			W.E. Acree, Jr.			
EIPERIMENTAL V	VALUES						
P/atm	<i>x</i> ₂	<i>x</i> ₁	P/atm	<i>x</i> ₂	<i>x</i> 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 \pm 0.1. x_1 : \pm 1-3 % at atmospheric pressure, and \pm 10 % at the higher pressures.

COMPONENTS:	OMPONENTS:		ORIGINAL P	ŒASUREMENTS:	 		
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		Djordjev	Djordjevic, N.M.				
(2) n-Octade	(2) n-Octadecane; C ₁₈ H ₃₈ ; [593-45-3]			Thermochim. Acta 1991, 177, 109-118.		him. Acta <u>1991</u> , 177, 109-118.	
VARIABLES:			PREPARED I	BY:			
Temperature			W.E. Acre	W.E. Acree, Jr.		W.E. Acree, Jr.	
EXPERIMENTAL	VALUES						
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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					
		AUXILI	ARY INFORMATION	ĭ			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
Differential	scanning cal		(1) Gold Label, 99+ %, Aldrich Chem Company, Milwaukee, Wisconsin, U used as received.		e, Wisconsin, USA, was		

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. Solubil-
ities determined by measuring melting
points of binary mixtures using a Perkin-
Elmer DSC-2 differential scanning calori-
meter and scan rate of 5 K/min.

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

ESTIMATED ERRORS:

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

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7] VARIABLES:			McLaughli	Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. J. Chem. Eng. Data 1985, 30, 403-409.			
			PREPARED BY:				
Temperature			W.E. Acre	e, Jr.			
EXPERIMENTAL V	/ALUES						
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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					
		AUXIL	ARY INFORMATION	ľ			
METHOD: APPARATUS/PROCEDURE			SOURCE AND	SOURCE AND PURITY OF MATERIALS:			

Constant temperature bath and a precision thermometer. $% \left(1\right) =\left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left($

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.

- 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 \pm 0.1. x_1 : \pm 0.0003.

COMPONENTS:

- (1) Phenanthrene; C14H10; [85-01-8]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]

EVALUATOR:

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

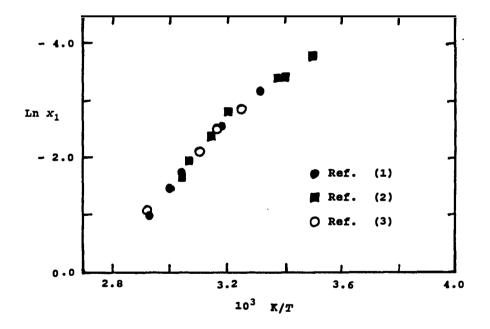
(USA)

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:

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

- McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 3854-3857. 1.
- 2. Gordon, L.J.; Scott, R.L. J. Am. Chem. Soc. 1952, 74, 4138-4140.
- Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. $J.\ Chem.\ Eng.\ Data\ 1985$, 30, 403-409. З.
- 4. Choi, P.B.; McLaughlin, E. AIChE J. 1983, 29, 150-153.

COMPONENTS:			ORIGINAL M	æasurements:			
(1) Phenanth	ene; C ₁₄ H ₁₀ ;	[85-01-8]	McLaughlin, E.; Zainal, H.A.				
(2) Cyclohexa	(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]			soc. <u>1960</u> ,	3854-3857.		
VARIABLES:			PREPARED E	PREPARED BY:			
Temperature			W.E. Acre	ee, Jr.			
EIPERIMENTAL \	VALUES	_					
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	N			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE ANI	D PURITY OF M	IATERIALS:		
Constant temperature bath and a precision thermometer.			(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			(2) Purity, source and purification method was not specified.				
noting the te		which the last	ESTIMATED	ERRORS:			
trace or son	ra solute dis	abbegren.		cision \pm 0.1.0003 (compile			

COMPONE	NTS:			ORIGINAL MEASUREMENTS:				
(1) Phe	enanthrene;	C14H10;	[85-01-8]	Gordon, L.J.; Scott, R.L.				
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7] VARIABLES:			J. Am. Chem. Soc. 1952, 74, 4138-4140.					
			PREPARED E	BY:				
Tempera	ature			W.E. Acre	ee, Jr.			
EXPERIME	ENTAL VALUE	S						
T/K	к <i>х</i>	2	<i>×</i> 1	T/K	x ₂	<i>x</i> ₁		
286	6.0 0	.9783	0.0217	317.6	0.9061	0.0939		
293	3.7 0	.9672	0.0328	326.7	0.856	0.144		
296	6.1 0	.9663	0.0337	328.2	0.827	0.173		
302	2.8 0	.9582	0.0418	341.9	0.596	0.404		
311	1.7 0	.9392	0.0608					
			AUXILIARY	INFORMATION	7			
ETHOD:	APPARATUS/I	PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer.			 White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, wa used as received. White Label, Eastman Kodak Chemical Company was used as received. 					
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								
determi	ned visuall	y by no	ting the temper- of solid solute	ESTIMATED	ERRORS:			
disappe	eared.	. –			ision \pm 0.2. nificant fig	ures (compiler).		

					= •		
COMPONENTS:			ORIGINAL I	MEASUREMENTS:			
(1) Phenanth	rene; C ₁₄ H ₁₀ ;	[85-01-8]	Coon, J.	E.; Auwaerter	, J.E.; McLaughlin, E.		
	(2) Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8]			Fluid Phase Equilibr. 1989, 44, 305-345.			
VARIABLES:	ARIABLES:		PREPARED I	BY:			
Temperature	Temperature		W.E. Acre	ee, Jr.			
EXPERIMENTAL V	VALUES						
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	* 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	1			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			wauke over then (2) 99+ % isome	ee, Wisconsin an activated recrystallizes, Aldrich Che er ratio of 6	hemical Company, Mil- t, USA, was passed alumina column and ed from solution. emical Company, having 0.6 % cis and 39.4 % r molecular sieves.		
	emperature at	which the last	ESTIMATED	ERRORS:			
			T/K: pred x ₁ : ± 0.0	cision ± 0.1. 003.			

COMPONENTS:	COMPONENTS:		ORIGINAL D	ORIGINAL MEASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Benzene; C ₆ H 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 E	Y:				
Temperature			W.E. Acre	e, Jr.				
EXPERIMENTAL V	ALUES		<u> </u>					
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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.
- lized from toluene.
 (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.0003.

COMPONENTS:	,		ORIGINAL N	EASUREMENTS:		
(1) Phenanthr	ene; C ₁₄ H ₁₀ ;	[85-01-8]	McLaughlin, E.; Zainal, H.A.			
(2) Benzene; C ₆ H ₆ ; [71-43-2]			J. Chem.	soc. 1959,	863-867.	
			PREPARED BY:			
Temperature	Temperature			ee, Jr.		
EXPERIMENTAL V	ALUES					
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	1		
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.			(1) Purity not specified, Bureau of Mines, USA, was passed over an alumina column with benzene as eluant.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		(2) "AnalaR", was dried over sodium wire and freshly distilled before use.				
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
CTACE OF BOIL	ra solute dis	ahhaar <i>an</i> ,		cision ± 0.1. 003 (compile:		

COMPONENTS:			ORIGINAL N	ORIGINAL MEASUREMENTS:				
(1) Phenanth	rene; C ₁₄ H ₁₀ ;	[85-01-8]	Speyers, C.L.					
(2) Methylbenzene; C ₇ H ₈ ; [108-88-3] VARIABLES:			Am. J. So	ei. <u>1902</u> , 14	1, 293-302.			
			PREPARED I	BY:				
Temperature			W.E. Acre	ee, Jr.				
EXPERIMENTAL \	ALUES		<u> </u>					
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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						
		AUXILIAR	Y INFORMATION	٧				
ETEOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:			
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing		talli point (2) Purit	 Purity not given, Kahlbaum, was recrystallized from toluene to a melting point temperature of 100.4 °C. Purity not given, Kahlbaum, was distilled before use. 					
the residue w	as subject to		ESTIMATED	ERRORS:				
				cision ± 0.1. (relative e	rror, compiler).			

			218
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Phenanthrene; C	4H ₁₀ ; [85-01-8]	Choi, P.B.; McLaughlin, E.	
(2) Methylbenzene; (C ₇ H ₈ ; [108-88-3]	AIChE J. <u>1983</u> , 29, 150-153.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	x ₂	<i>x</i> 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:

- 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 \pm 0.05. x_1 : \pm 0.0001 (Compiler).

COMPONENTS:			ORIGINAL 1	œasur ement s:	1	
(1) Phenanth	rene; C ₁₄ H ₁₀ ;	[85-01-8]	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E			
(2) 1,2,3,4-Tetrahydronaphthalene; C ₁₀ H ₁₂ ; [119-64-2]		Fluid Phase Equilibr. 1989, 44, 305-345.				
VARIABLES:			PREPARED E	Y:		
Temperature	Temperature			W.E. Acree, Jr.		
EXPERIMENTAL '	VALUES					
T/K	x ₂	<i>x</i> ₁	T/K	x 2	<i>x</i> 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	ī		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed		(1) 98.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.				
in glass amportemperature t	oules and pla	ced in constant	(2) 99.64 store	%, Aldrich	Chemical Company, was cular sieves to remove	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Rai, U.S.; Shekhar, H.
(2) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Thermochim. Acta <u>1991</u> , 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 $x_1 = 0.23$ and T/K = 333.7.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter and an analytical balance.

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.

Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques.

SOURCE AND PURITY OF MATERIALS:

trace water.
ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.0003.

- (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 M	Easurements:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Kravchenko	o, V.M.; Pastukhova, I.S.
(2) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]		nem. U.S.S.R. <u>1959</u> , 29, 29-34. translation)
VARIABLES:	PREPARED BY	ľ:
Temperature	W.E. Acree	e, Jr.
EXPERIMENTAL VALUES		
<i>T</i> /K	* 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) 0.437 (2) 353.4 0.563 347.5 0.480 0.520 (2) 346.2 0.460 0.540 Eutectic 349.6 0.391 0.609 (1) 0.706 355.3 0.294 (1) (1) 363.8 0.156 0.844 (1) 368.7 0.065 0.935 1.000 372.5 0.000 (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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] VARIABLES:		Kravchenko	Kravchenko, V.M.; Pastukhova, I.S. Zhur. Fiz. Khim. 1957, 31, 1802-1811. PREPARED BY:			
		Zhur. Fiz.				
		PREPARED BY				
Temperature		W.E. Acree	W.E. Acree, Jr.			
EXPERIMENTAL VALUES			G-1/3 Bh			
T/K	x ₂	× 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)			
		ARY INFORMATION				
Phase diagram was detthermal analysis methodetail in V.M. Kravch. U.S.S.R. 1939, 13, 1: visual observations.	ermined using a od (described in enko, J. Phys. Chem	(1) Purity specifi before y	and chemical source were not ed in paper, was recrystallized			

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Tetrachloromethane; CCl ₄ ; [56-23-5] VARIABLES:		McLaughlin, E.; Zainal, H.A.				
		J. Chem. Soc. <u>1960</u> , 2485-2488.				
		PREPARED BY:				
Temperature	rature		W.E. Acree, Jr.			
EXPERIMENTAL	VALUES		<u> </u>			
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	N		
METHOD: APPARATUS/PROCEDURE		SOURCE AND	D PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		Unite	ed Kingdom, w	British Drug Hous as passed over an th benzene as eluar	-	
		(2) AnalaR grade, source not givne, was stored over anhydrous calcium chloride and distilled before use.			lde	
noting the temperature at which the last trace of solid solute disappeared.			ESTIMATED	ERRORS:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Rai, U.S.; Shekhar, H.
(2) 1,4-Dibromobenzene; C ₆ H ₄ Br ₂ ; [106-37-6]	Thermochim. Acta <u>1991</u> , 175, 215-227.
VARIABLES:	PREPARED BY:
	W.E. Acree, Jr.

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

EXPERIMENTAL VALUES

Phase diagram, given in the orignal 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					
SOURCE AND PURITY OF MATERIALS:					
(1) Purity not given, Thomas Backer & Co., Bombay, India, was purified by frac- tional recrystallization from ethanol.					
(2) Purity not given, Fluka AG, Switzer- land, was purified by crystallization from boiling 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]	McLaughlin, E.; Scott, R.L.				
(2) 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7- pentadecafluoroheptane; C ₇ HF ₁₅ ; [375-83-7]	J. Phys. Chem. <u>1956</u> , 60, 674-676.		J. Phys. Chem. <u>1956</u> , 60, 674-676.		
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EIPERIMENTAL VALUES					
t/K x ₂	<i>x</i> ₁				
25.0 0.9984	0.00160				
AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, a precision thermometer and uv/visible spectrometer. Mixtures of known concentrations sealed	(1) White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, was recrystallized ten times from ethanol.				
in glass ampoules and allowed to equili- brate at a constant temperature for an unspecified length of time. Solubilities calculated from spectral absorbance data	(2) Purity not specified, synthesized by authors, was fractionally distilled shortly before use.				
at 270 nm.	ESTIMATED ERRORS:				
	T/K : precision \pm 0.01. x_1 : \pm 3 % (relative error; compiler).				

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		85-01-8]	McLaughlin, E.; Scott, R.L.				
(2) 1,1,2,2 hexadeca [307-99-	,3,3,4,4,5,5,6, afluorooctane; -3]	6,7,7,8,8- C ₈ H ₂ F ₁₆ ;	J. Phys. Chem. <u>1956</u> , 60, 674-676.				
VARIABLES:			PREPARED BY:				
T/K = 298			W.E. Acree, Jr.				
EXPERIMENTAL	VALUES						
t/	/ K	x ₂	<i>x</i> ₁				
25.0 0.9951			0.00488				
		AUXILIAR	Y INFORMATION				
ŒTHOD: APPAR	RATUS/PROCEDURE		Y INFORMATION SOURCE AND PURITY OF MATERIALS:				
Constant tem	perature bath, and uv/visible	a precision spectrometer.					
Constant tem thermometer Mixtures of in glass amp brate at a c unspecified	nperature bath, and uv/visible known concentr coules and allo	a precision spectrometer. ations sealed wed to equili- ature for an . Solubilities	SOURCE AND PURITY OF MATERIALS: (1) White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, wa				

T/K: precision \pm 0.01. x_1 : \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Phenanthrene; C₁₄H₁₀; [85-01-8] Octafluoronaphthalene; C₁₀F₈; [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 (1) Purity not given, Tokyo Chemical analytical balance. Company, Japan, was zone-refined before Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential (2) Reagent grade, Tokyo Chemical Company, Japan, was recrystallized from methscanning calorimetric techniques. anol before use. ESTIMATED ERRORS: T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.02 (Compiler).

COMPONENTS:		ORIGINAL I	ORIGINAL MEASUREMENTS:			
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Ethanol; C ₂ H ₆ O; [64-17-5]		Speyers,	Speyers, C.L. Am. J. Sci. <u>1902</u> , 14, 293-302.			
		Ат. J. S				
VARIABLES:			PREPARED 1	BY:		
Temperature	Temperature		W.E. Acre	W.E. Acree, Jr.		
EXPERIMENTAL	VALUES					
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	x ₁	
273.2	0.9918	0.0082	320.2	0.9781	0.0219	
284.1	284.1 0.9914 0.0086		343.4	0.9248	0.0752	
305.3	305.3 0.9844 0.0156					
305.3	0.3044	0.0150				

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

ESTIMATED ERRORS:

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

ORIGINAL MEASUREMENTS:
Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. 1985, 19, 522-529.
PREPARED BY:
W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C

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

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:

- 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: \pm 0.1 (compiler). c₁: \pm 3 % (relative error; compiler).

PONENTS: ORIGIN			RIGINAL MEASUREMENTS:			
1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		Choi, P.	Choi, P.B.; McLaughlin, E.			
C5H5N; [110	-86-1]	Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-5				
		PREPARED I	PREPARED BY:			
		W.E. Acre	W.E. Acree, Jr.			
ALUES		· ·				
<i>x</i> ₂	* 1	T/K	<i>x</i> ₂	<i>x</i> ₁		
0.7541	0.2459	342.8	0.3830	0.6170		
0.6989	0.3011	349.6	0.3039	0.6961		
0.6487	0.3513	355.6	0.2349	0.7651		
0.6310	0.3690	361.0	0.1651	0.8349		
0.5717	0.4283	366.5	0.0889	0.9111		
	C ₅ H ₅ N; [110-	C ₅ H ₅ N; [110-86-1] ALUES *2 *1 0.7541 0.2459 0.6989 0.3011 0.6487 0.3513 0.6310 0.3690	Total C ₅ H ₅ N; [110-86-1] Ind. Eng PREPARED I W.E. Acro ALUES X ₂ X ₁ 0.7541 0.2459 0.6989 0.3011 349.6 0.6487 0.3513 355.6 0.6310 0.3690 361.0	Total C5H5N; [110-86-1] Ind. Eng. Chem. Funda PREPARED BY: W.E. Acree, Jr. ALUES X2		

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:

- 98.7 %, Eastern Chemical Company, Smithtown, New York, USA, was passed over activated alumina and then recrystallized from toluene.
- lized from toluene.
 (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision \pm 0.1. x_1 : \pm 0.0003.

					,22					
COMPONENTS: (1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Thiophene; C ₄ H ₄ S; [110-02-1] VARIABLES: Temperature		ORIGINAL	Measurements:							
		Choi, P.B.; McLaughlin, E. Ind. Eng. Chem. Fundam. 1983, 22, 46-51. PREPARED BY: W.E. Acree, Jr.								
					EXPERIMENTAL '	VALUES				
					T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	N						
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	ATERIALS:					
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly		town, activ lized (2) Gold	, New York, U vated alumina I from toluen Label, 99.9+	themical Company, Smith- SA, was passed over and then recrystal- e. %, Aldrich Chemical as received.						
noting the te	increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.		T/K: pred x ₁ : ± 0.0	cision ± 0.1.						

(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:		PREPARED BY:
					T/K = 298, 308 and 318		W.E. Acree, Jr.
EXPERIMENTAL VALUES		<u> </u>					
t/K	<i>x</i> ₂	x ₁					
25.0	0.9708	0.0292					
35.0	0.9511	0.0489					
45.0	0.9278	0.0722					

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:

- White Label, Eastman Kodak Chemical Company, Rochester, New York, USA, was recrystallized five times from ethanol to give a melting point of 101 °C.
 Purity not specified, Minnesota Mining
- (2) Purity not specified, Minnesota Mining & Manaufacturing Company, USA, was distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision \pm 0.02. x_1 : \pm 2 % (relative error; compiler).

residue.

COMPONENTS:			ORIGINAL I	EASUREMENTS:		
COMPOREMIS:		ORIGINAL REASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]			Srivastava, R.D.; Gupta, P.D.			
(2) Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3] VARIABLES: Temperature		J. India	n Chem. Soc.	<u>1967</u> , 44, 960-963.		
		PREPARED I	BY:			
		W.E. Acree, Jr.				
EXPERIMENTAL V	VALUES		ļ			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	4		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.		Unite	ty not given, ed Kingdom, w imed.	British Drug Houses, as recrystallized and		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual						
noting the te	emperature at	which the last	ESTIMATED	ERRORS:	•	
trace of soli	trace of solid solute disappeared.			cision ± 0.1. (relative e	rror, Compiler).	

COMPONENTS: (1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]			ORIGINAL MEASUREMENTS: Doane, E.P.; Drickamer, H.G. J. Phys. Chem. 1955, 59, 454-457. PREPARED BY: W.E. Acree, Jr.							
						(2) Carbon disulfide; CS ₂ ; [75-15-0] VARIABLES: T/K = 298, Pressure				
EXPERIMENTAL	VALUES							<u> </u>		
P/atm	x ₂	x ₁						P/atm	x ₂	<i>x</i> 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	ľ						
ŒTHOD: APPAR	ATUS/PROCEDU	RE	SOURCE AND	PURITY OF	MATERIALS:					
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,		(1) Purest grade, Eastman Kodak Chemical Company, Rochester, New York, USA, w used as received.		er, New York, USA, was						
		(2) C.P. grade, J.T. Baker, was dried over phosphorous pentoxide and distilled.								
solvent evap	orated to dry	rness, and con- reight of solid	ESTIMATED	ERRORS:						
residue.			T/V. procision + 0 1							

T/K: precision \pm 0.1. x_1 : \pm 1-3 % at atmospheric pressure, and \pm 10 % at the higher pressures.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Kremann, R.
(2) 1,2-Dinitrobenzene; C ₆ H ₄ N ₂ O ₄ ; [528-29-0]	Monatsch. Chem. 1908, 29, 863-890.
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EIPERIMENTAL VALUES	

NTAL VALUES			
T/K	x ₂	<i>*</i> 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

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:

COMPONENTS	:		ORIGINAL MEASUREMENTS:		
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		[85-01-8]	Kremann, R. Monatsch. Chem. 1908, 29, 863-890.		
(2) 1,3-D [99-6	(2) 1,3-Dinitrobenzene; C ₆ H ₄ N ₂ O ₄ ; [99-65-0]				
VARIABLES:			PREPARED BY:		
Temperatu	re		W.E. Acree, Jr.		
EXPERIMENT.	AL VALUES				
T/K	* ₂	x ₁	<i>T/</i> K		
362.7	1.000	0.000	362.2 0.179 0.821		
360.2	0.955	0.045	369.2 0.103 0.897		
356.2	0.900	0.100	373.2 0.048 0.952		
353.2	0.847	0.153	376.7 0.000 1.000		
349.7	0.806	0.194	Compiler. Entertie seint comment		
345.2	0.753	0.247	Compiler: Eutectic point occurs at about $x_1 = 0.482$ and $T/K = 320.6$.		
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			
		AUXII	LIARY 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:

COMPONENTS: (1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) 1,4-Dinitrobenzene; C ₆ H ₄ N ₂ O ₄ ; [100-25-4]		ORIGINAL ME	Asurements:	
		Kremann, R. Monatsch. Chem. <u>1908</u> , 29, 863-890.		
Temperature	Temperature		, Jr.	
EIPERIMENTAL VALUES				
T/K	x ₂	× 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)	
	Allett	IARY 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:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Phenanthrene; C₁₄H₁₀; [85-01-8] Kremann, R. (2) 1,3,5-Trinitrobenzene; C₆H₃N₃O₆; [99-35-4] Monatsch. Chem. 1908, 29, 863-890. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K X₁ x_2 394.2 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

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:

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) 1,2,3,5-Tetranitrobenzene; C ₆ H ₂ N ₄ O ₈ ; [3698-53-1] VARIABLES: Temperature		Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270. 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)			
			(1) 1:1 phenanthrene - 1,2,3,5-			

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	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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).				

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Phenanthrene; C₁₄H₁₀; [85-01-8] Kremann, R. Monatsch. Chem. 1908, 29, 863-890. (2) 2,4-Dinitro-1-methylbenzene; C7H6N2O4; [121-14-2] PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K T/K X1 x₂ x₂ ×1 0.293 0.707 1.000 0.000 351.2 342.2 0.738 341.2 0.968 0.032 354.7 0.262 0.790 360.2 0.210 338.7 0.924 0.076 365.7 0.151 0.849 337.2 0.889 0.111 0.878 334.7 0.854 0.146 368.2 0.122 0.076 0.924 0.819 371.2 333.2 0.181 0.209 376.7 0.000 1.000 0.791 331.2 329.2 0.756 0.244 Compiler: Eutectic point occurs at about $x_1 = 0.447$ and T/K = 310.6. 327.7 0.733 0.267 0.284 326.2 0.716 0.693 0.307 324.2 322.2 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 0.529 326.2 0.471 332.7 0.427 0.573 0.402 0.598 336.2 0.372 0.628 341.2 0.334 0.666 346.7

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:

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

ESTIMATED ERRORS:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Phenanthrene; C₁₄H₁₀; [85-01-8] Kremann, R. Monatsch. Chem. 1908, 29, 863-890. (2) 2,6-Dinitro-1-methylbenzene; C7H6N2O4; [606-20-2] VARTARIRE. PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x_2 x_1 338.2 1.000 0.000 (2) 0.979 0.021 (2) 337.2 333.7 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) 0.620 345.2 0.380 (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) 0.088 370.4 0.912 (1) 373.7 0.048 0.952 (1) 376.7 0.000 1.000 (1)

AUXILIARY INFORMATION

Compiler: Eutectic point occurs at about $x_1 = 0.375$ and T/K = 311.7.

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:

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

ESTIMATED ERRORS:

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) 3,4-Dinitro-1-methylbenzene; C ₇ H ₆ N ₂ O ₄ ; [610-39-9] VARIABLES: Temperature		Kremann, R. Monatsch. Chem. 1908, 29, 863-890.	
		W.E. Acree, Jr.	
		EXPERIMENTAL VALUES	
T/K	x ₂	<i>x</i> 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)
	0.060	0.940	(1)
372.7			

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:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Phenanthrene; C₁₄H₁₀; [85-01-8] Kremann. R. Monatsch. Chem. 1908, 29, 863-890. (2) 2,4,6-Trinitro-1-methylbenzene; C₇H₅N₃O₆; [118-96-7] PREPARED BY: VARIARIES. Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K ×2 x₁ 351.2 1.000 0.000 (2) 347.2 0.896 0.104 (2) 0.828 0.172 (2) 343.2 345.2 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 1:1 Compound 360.7 0.483 0.517 360.2 0.459 0.541 1:1 Compound 1:1 Compound 359.7 0.444 0.556 0.406 1:1 Compound 358.0 0.594 0.371 0.629 1:1 Compound 355.2 0.342 0.658 1:1 Compound 352.2 0.678 1:1 Compound 350.7 0.322 350.2 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) 0.072 0.928 371.7 (1) 0.041 0.959 374.7 (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.

1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

376.7

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.

0.000

SOURCE AND PURITY OF MATERIALS:

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

(1)

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

ESTIMATED ERRORS:

COMPONENTS: ORIGINAL MEASUREMENTS: Kremann, R.; Hofmeier, F. (1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) 2,4-Dinitrophenol; C₆H₄N₂O₅; [51-28-5] Monatsch. Chem. 1910, 31, 201-202. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x₂ x₁ 1.000 0.000 384.2 (2) 0.970 0.030 382.2 (2) 380.2 0.928 0.072 (2) 377.2 0.872 0.128 (2) 0.845 0.155 374.2 (2) 0.203 371.2 0.797 (2) 369.2 0.755 0.245 (2) 0.282 366.2 0.718 (2) 363.2 0.677 0.323 (2) 360.2 0.641 0.359 (2) 0.595 0.405 355.2 (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) 0.376 341.2 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 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 \pm 0.5 (Compiler).

 x_1 : \pm 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) 1-Chloro-4-nitrobenzene; C ₆ H ₄ ClNO ₂ ; [100-00-5]	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.

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. (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). x1: ± 0.01 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthene; C ₁₄ H ₁₀ ; [85-01-8]	Burger, A.; Bryant, H.W.
(2) Dibenzothiophene; C ₁₂ H ₈ S; [132-65-0]]	J. Am. Chem. Soc. 1941, 63, 1054-1057.
VARIABLES:	PREPARED BY:
Temperature	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.

AUXILIA	RY INFORMATION
ETHOD: 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 \pm 0.2 (Compiler). x_1 : \pm 0.01 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Thianthrene; C ₁₂ H ₈ S ₂ ; [92-85-3] VARIABLES: Temperature		Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; Eckert, C.A. J. Chem. Eng. Data 1990, 35, 446-449.	
		PREPARED BY: W.E. Acree, Jr.	
			EXPERIMENTAL VALUES
T/K	* ₂	<i>*</i> 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)

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 \pm 0.5. x_1 : \pm 0.005 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Rai, U.S.; Shekhar, H.
(2) Benzoic Acid; C ₇ H ₆ O ₂ ; [65-85-0]	Cryst. Res. Technol. <u>1990</u> , 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.

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. (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). x1: ± 0.01 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Rai, U.S.; Shekhar, H.
(2) trans-Cinnamic Acid; C ₇ H ₆ O ₂ ; [140-10-3]	Cryst. Res. Technol. 1990, 25, 771-779.
VARIABLES:	PREPARED BY:
	W.E. Acree, Jr.
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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:

COMPONENTS: ORIGINAL MEASUREMENTS: Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; (1) Phenanthrene; C, H, 10; [85-01-8] Eckert, C.A. (2) 2-Hydroxybenzoic acid; C₇H₆O₃; [69-72-7] J. Chem. Eng. Data 1990, 35, 446-449. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x_1 $\boldsymbol{x_2}$ 1.00 0.00 (2) 432 0.90 0.10 423 (2) 416 0.80 0.20 (2) 0.70 0.30 410 (2) 404 0.60 0.40 (2) 0.50 0.50 398 (2) 0.60 390 0.40 (2) 0.30 0.70 381 (2) 368 0.20 0.80 (2) 0.10 0.90 367 (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. 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:

- 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 \pm 0.5. x_1 : \pm 0.005 (Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:	
 Phenanthrene; C₁₄H₁₀; [85-01-8] 3-Hydroxybenzoic acid; C₇H₆O₃; [99-06-9] 		Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; Eckert, C.A. J. Chem. Eng. Data 1990, 35, 446-449.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES		!	
T/K	* ₂	<i>x</i> 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. 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 \pm 0.5. x_1 : \pm 0.005 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Efremov, N.N.; Fikhomirova, A.N.
(2) 6-Methyl-2,3,4-trinitrophenol; C ₇ H ₅ N ₃ O ₇ ; [89793-90-8]	J. Russ. Phys. Chem. Soc. <u>1927</u> , 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

AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Experimental details not given in paper. determined using a Toshiniwal Melting Point Apparatus equipped with a precision thermometer.	(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. <u>Alkenes</u>
- C. Aromatic Hydrocarbons
- D. Esters
- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. Alcohols
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>
- J. Binary Solvent Mixtures

methanol + water
ethanol + water

EXPERIMENTAL VALUES

COMPONENTS: (1) 1,10-Phenanthroline; C ₁₂ H ₈ N ₂ ; [5144-89-8] (2) Methanol; CH ₄ O; [67-56-1] (3) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Burgess, J.; Haines, R.I. J. Chem. Eng. Data 1978, 23, 196-197.
VARIABLES: T/K = 298, Solvent composition	PREPARED BY: W.E. Acree, Jr.

t = 25.0	°C	
	φ ₂ (s)	$c_1/(\text{mol dm}^{-3})$
Ī	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:

- Purity and chemical source not specified, was recrystallized from aqueousethanol.
- (2) Purity and chemical source not specified in paper.
- (3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: \pm 0.1 (Compiler). $\phi_2^{(s)}$: \pm 0.01 (Compiler). c_1 : \pm 3 % (relative error, Compiler).

	24
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,10-Phenanthroline; C ₁₂ H ₈ N ₂ ; [5144-89-8]	Sengupta, D.; Amalendu, P.; Lahiri, S.C.
(2) Methanol; CH ₄ O; [67-56-1] (3) Water; H ₂ O; [7732-18-5]	J. Chem. Soc., Dalton Trans. <u>1983</u> , 2685- 2688.
variables:	PREPARED BY:
T/K = 295, Solvent composition	W.E. Acree, Jr.
EIPERIMENTAL VALUES ^a t = 22.0 °C	
*2 ^(s)	$c_1/(mol dm^{-3})$
0.000	0.0169
0.047	0.0269

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

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures prepared volume-trically 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 speci-fied in paper.

ESTIMATED ERRORS:

T/K: \pm 0.1 (Compiler). $x_2^{(s)}$: \pm 0.001 (Compiler). c_1 : \pm 3 % (relative error, Compiler).

 $^{^{}a}$ $x_{2}^{(s)}$: 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.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 1,10-Phenanthroline; C₁₂H₈N₂; [5144-89-8] Ethanol; C₂H₆O; [64-17-5] Water; H₂O; [7732-18-5] 	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	
*2 ^(s)	$c_1/(\text{mol dm}^{-3})$
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 volume-trically 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:

 $T/K_1 \pm 0.1$ (Compiler). $x_2^{(s)} : \pm 0.001$ (Compiler). $c_1 : \pm 3$ % (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. <u>Ketones</u>
- I. Miscellaneous Pure Solvents

phenoxazine
thianthrene
phenoxanthiin
dibenzo[b,e][1,4]dioxine

J. Binary Solvent Mixtures

COMPONENTS:		ORIGINAL MEA	ORIGINAL MEASUREMENTS:		
(1) Phenothiazine; C ₁₂ H ₉ NS; [92-84-2]		Cullinane,	Cullinane, N.M.; Rees, W.T.		
(2) Phenoxazine; C ₁₂ H ₉	2) Phenoxazine; C ₁₂ H ₉ NO; [135-67-1]		day Soc. <u>1940</u> , 36, 506-514.		
VARIABLES:		PREPARED BY:			
Temperature			Jr.		
EXPERIMENTAL VALUES ^a					
T _{in} /K	T _{fin} /K	* 2	× 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		

⁸ 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 $x_2 = 1.00$. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

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:

- 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:

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Phenothiazine; C ₁	(1) Phenothiazine; C ₁₂ H ₉ NS; [92-84-2] (2) Thianthrene; C ₁₂ H ₈ S ₂ ; [92-85-3]		Cullinane, N.M.; Rees, W.T.			
(2) Thianthrene; C ₁₂ H ₈			Trans. Faraday Soc. <u>1940</u> , 36, 506-514.			
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acree,	Jr.			
EXPERIMENTAL VALUES ⁸						
$T_{\sf in}/{\sf K}$	T _{fin} /K	* ₂	<i>×</i> 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 $x_1=1.00$. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

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:

- 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:

COMPONENTS:		ORIGINAL MEAS	SUREMENTS:
(1) Phenothiazine; C ₁₂	H ₉ NS; [92-84-2]	Cullinane, 1	N.M.; Rees, W.T.
(2) Phenoxanthiin; C ₁₂	H ₈ OS; [262-20-4]	Trans. Farac	day Soc. 1940, 36, 506-514.
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree,	Jr.
EXPERIMENTAL VALUES			
T _{in} /K	T _{fin} /K	x ₂	<i>x</i> 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
1			

^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. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

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:

- 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:

COMPONENTS:			ORIGINAL MEASUR	ements:		
(1) Phenothi	1) Phenothiazine; C ₁₂ H ₉ NS; [92-84-2]		Cullinane, N.M.; Rees, W.T.			
(2) Dibenzo[[262-12-	<pre>2) Dibenzo[b,e][1,4]dioxin; C₁₂H₈O₂; [262-12-4]</pre>			Trans. Faraday Soc. <u>1940</u> , 36, 506-514.		
VARIABLES:			PREPARED BY:			
Temperature			W.E. Acree, Jr.			
EIPERIMENTAL	VALUES					
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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: APPAR	ATUS/PROCEDUI	RE	SOURCE AND PURI	TY OF MATERIA	ALS:	
tubes. Temp with ample to Transition to visual observations	erature was s ime given for emperatures o vations. Rep	small capillary slowly varied equilibration. determined by corted tempera- tive measurements.	sublimation alcohol. (2) Purity and	in paper, was n and recryst chemical sou recrystalli	urce were not s purified by tallization from urce not given, ization from	
			ESTIMATED ERRORS	S:		
			T/K : precision x_1 : \pm 0.002 (Co		iler).	

PHENOXANTHIIN SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

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

phenoxazine
thianthrene
phenothiazine
dibenzo[b,e][1,4]dioxin

J. Binary Solvent Mixtures

COMPONENTS:			ORIGINAL MEASUR	EXENTS:		
(1) Phenoxan	thiin; C. H.O	S; [262-20-4]	Cullinane, N.M.; Rees, W.T.			
	(2) Phenoxazine; C ₁₂ H ₈ NO; [135-67-1]			Trans. Faraday Soc. 1940, 36, 506-514.		
	RIABLES:			PREPARED BY:		
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL '	VALUES		•			
T/K	* ₂	<i>x</i> ₁	T/K	x ₂	* 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: APPARA	ATUS/PROCEDUI	RE	SOURCE AND PURI	TY OF MATERIA	ALS:	
tubes. Tempe with ample to Transition to visual observ	erature was s ime given for emperatures c vations. Rep	small capillary slowly varied equilibration. determined by corted tempera- cive measurements.	fied by red and sublimate (2) Synthesized	crystallizati ation. d by authors, blimation and	, and was puri- ion from alcohol , and was puri- i recrystallized	
			ESTIMATED ERRORS	5:		
			T/K : precision x_1 : \pm 0.002 (Co		ller).	

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Phenoxan	1) Phenoxanthiin; C ₁₂ H ₈ OS; [262-20-4] 2) Thianthrene; C ₁₂ H ₈ S ₂ ; [92-85-3] RIABLES:		Cullinane, N.M.; Rees, W.T.			
(2) Thianthre			Trans. Faraday	soc. <u>1940</u> ,	36, 506-514.	
VARIABLES:			PREPARED BY:			
Temperature			W.E. Acree, Jr.	•		
EXPERIMENTAL V	/ALUES					
T/K	<i>x</i> ₂	<i>*</i> 1	T/K	x ₂	<i>x</i> 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	

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported tempera-

tures verified by repetitive measurements.

Synthesized by the authors, was purified by sublimation and recrystallized from alcohol.

(2) Purity and chemical source not given, was purified by sublimation and recrys-tallization from acetone.

ESTIMATED ERRORS:

COMPONENTS:	OMPONENTS:		SUREMENTS:	
1) Phenoxanthiin; C ₁₂ H ₈ OS; [262-20-4]		Cullinane, N.M.; Rees, W.T.		
(2) Phenothiazine; C ₁₂ H ₉	Phenothiazine; C ₁₂ H ₉ NS; [92-84-2]		day Soc. <u>1940</u> , 36, 506-514.	
ARIABLES:		PREPARED BY:		
Temperature		W.E. Acree,	Jr.	
EXPERIMENTAL VALUES				
r_{in}/κ	$T_{\sf fin}/{\sf K}$	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. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

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:

- 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:

COMPONENTS:			ORIGINAL MEASUR	EMENTS:		
(1) Phenoxan	thiin; C ₁₂ H ₀ C	s; [262-20-4]	Cullinane, N.M.; Rees, W.T.			
	(2) Dibenzo[b,e][1,4]dioxin; C ₁₂ H ₈ O ₂ ; [262-12-4]			Trans. Faraday Soc. 1940, 36, 506-514.		
VARIABLES:			PREPARED BY:			
Temperature	mperature			W.E. Acree, Jr.		
EXPERIMENTAL '	VALUES		<u>:</u>			
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		SOURCE AND PURI	TY OF MATERIA	ALS:		
tubes. Tempe with ample to Transition to visual observ	erature was dime given for emperatures divations. Rej	small capillary slowly varied r equilibration. determined by ported tempera- cive measurements.	fied by real and sublimated (2) Purity and fied in page	crystallizat: ation. chemical so	, and was puri- ion from alcohol urce not speci- d by sublimation acetone.	

ESTIMATED ERRORS:

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

phenothiazine
phenoxanthiin
thianthrene
dibenzo[b,e][1,4]dioxin

J. Binary Solvent Mixtures

				200
COMPONENTS:		ORIGINAL MEA	SUREMENTS:	
(1) Phenoxazine; C ₁₂ H ₅	,NO; [135-67-1]	Cullinane,	N.M.; Rees, W.T.	
(2) Phenothiazine; C ₁	2 ^H 9NS; [92-84-2]	Trans. Fara	day Soc. <u>1940</u> , 36, 506-514.	
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree,	Jr.	
EXPERIMENTAL VALUES ⁸				
τ _{in} /κ	T _{fin} /K	x ₂	<i>x</i> 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 $x_1 = 1.00$. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

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:

- 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:

COMPONENTS:			ORIGINAL MEASUREMENTS: Cullinane, N.M.; Rees, W.T.			
(1) Phenoxazi	ine; C ₁₂ H ₀ NO;	[135-67-1]				
(2) Phenoxanthiin; C ₁₂ H ₈ OS; [262-20-4]		Trans. Faraday	Soc. 1940,	<i>36</i> , 506-514.		
ARIABLES:			PREPARED BY:			
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL \	VALUES		<u></u>			
T/K	x ₂	<i>*</i> 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			
ETHOD: APPARA	ATUS/PROCEDUE	RE	SOURCE AND PURIT	TY OF MATERIA	ALS:	
with ample to Transition to visual observ	erature was s ime given for emperatures d vations. Rep	small capillary slowly varied equilibration. letermined by corted tempera- cive measurements.	(2) Synthesized by authors, and was fied by sublimation and recrysta			
			ESTIMATED ERRORS	3:		
			T/K: precision x ₁ : ± 0.002 (Co		iler).	

COMPONENTS:	COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Phenoxazine; C ₁₂ H ₉ NO; [135-67-1]		Cullinane, N.M.; Rees, W.T.				
(2) Thianthr	ene; C ₁₂ H ₈ S ₂ ;	[92-85-3]	Trans. Faraday	soc. <u>1940</u> ,	<u>1940</u> , <i>36</i> , 506-514.	
VARIABLES:			PREPARED BY: W.E. Acree, Jr.		<u> </u>	
Temperature						
EIPERIMENTAL	VALUES		<u>. </u>			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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				

| |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:

- 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:

				20			
COMPONENTS: (1) Phenoxazine; C ₁₂ H ₉ NO; [135-67-1] (2) Dibenzo[b,e][1,4]dioxin; C ₁₂ H ₈ O ₂ ; [262-12-4] VARIABLES: Temperature		ORIGINAL MEASUREMENTS:					
		Cullinane, N.M.; Rees, W.T. Trans. Faraday Soc. 1940, 36, 506-514. PREPARED BY:					
					W.E. Acree, Jr.		
					EIPERIMENTAL VALUES ^a		
		T _{in} /K	T _{fin} /K	x ₂	<i>x</i> 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	ļ			
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 $x_1 = 1.00$. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

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:

- 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:

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

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. <u>Ketones</u>

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-dinitromethylbenzene
2,4,6-trinitromethoxybenzene
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-octane + 2-propanol
cyclohexane + 2-propanol
methylcyclohexane + 2-propanol
2,2,4-trimethylpentane + 2-propanol

200			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [12 (2) n-Hexane; C ₆ H ₁₄ ; [13		Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr. J. Chem. Eng. Data 1987, 32, 60-62. PREPARED BY:	
VARIABLES:			
T/K = 299		W.E. Acree, Jr.	
EXPERIMENTAL VALUES		•	
t/° C	x 2	x ₁	
26.0	0.9915	0.00852	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature in thermometer, and an use spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.		(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
		ESTIMATED ERRORS:	
		T/K : \pm 0.05. x_1 : \pm 1 % (relative error).	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]		Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.
(2) ii neptane, 07.116, [142	52 5 ,	J. Chem. Eng. Data <u>1987</u> , 32, 60-62.
VARIABLES:		PREPARED BY:
T/K = 299		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/° C	<i>x</i> ₂	x ₁
26.0	0.9890	0.01101
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	3	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.		(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
		ESTIMATED ERRORS:
		T/K : \pm 0.05. x_1 : \pm 1 % (relative error).

	26
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Lissi, E.A.; Abuin, E.B.
(2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]	Bol. Soc. Chil. Quim. 1981, 26, 19-34.
Variables:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C	(mol dm ⁻³)
20.0 0.0	0120
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.
Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane	(2) Purity and chemical source not given, purification procedure not specified.
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 extra- polates up to saturation point.	ESTIMATED ERRORS:
	T/K : ± 2 . c_1 : unknown.

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) n-Octane; C ₈ H ₁₈ ; [111-65-9]		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	0.9862	0.01379	
 :	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.		(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: Djordjevic, N.M.			
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) n-Octadecane; C ₁₈ H ₃₈ ; [593-45-3]					
			Thermochim. Acta 1991, 177, 109-118.		
VARIABLES:			PREPARED BY:		
Temperature		W.E. Acre	ee, Jr.		
EXPERIMENTAL '	VALUES				
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	ı	
METHOD: APPAR	METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:
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.		(1) 99+ % wauke recei	e, Wisconsin	emical Company, Mil- , USA, was used as	
		(2) 99 %, vacuu	Aldrich Chemmedistilled	mical Company, was before use.	
		ESTIMATED	ERRORS:		
			cision ± 0.3 003 (compile:		

	ORIGINAL MEASUREMENTS:	
	Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr. J. Chem. Eng. Data 1987, 32, 60-62.	
	PREPARED BY:	
	W.E. Acree, Jr.	
* ₂	<i>x</i> ₁	
0.9891	0.01089	
0.9691	0.01069	
	-	

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:

- 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: \pm 0.05. x_1 : \pm 1 % (relative error).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		ORIGINAL MEASUREMENTS:	
		McLaughlin, E.; Zainal, H.A.	
		J. Chem. Soc. <u>1960</u> , 3854-3857.	
VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	x ₂	<i>x</i> 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		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath and a precision thermometer.		(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.		(2) Purity, source and purification method was not specified.	
		ESTIMATED ERRORS:	
		T/K: precision \pm 0.1. x_1 : \pm 0.0003 (compiler).	

COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		ORIGINAL MEASUREMENTS:	
		Carre, O.R.; Phillips, D.J.; Brennecke, J.F.	
		Ind. Eng. Chem. Res. 1994, 33, 1355-1362.	
VARIABLES:		PREPARED BY:	
T/K = Circa 294 (Ambient Room)		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/° C	x ₂	<i>x</i> ₁	
21.0	0.9886	0.0114	
AUXILIARY METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE Ultraviolet/visible spectrophotometer and centrifugal automatic particle anal-		SOURCE AND PURITY OF MATERIALS: (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.	
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.		(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 ₇ H 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.	
T/K = 299			
EXPERIMENTAL VALUES		•	
t/° C	x ₂	x ₁	
26.0	0.9870	0.0130	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.		(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
		ESTIMATED ERRORS:	
		T/K: ± 0.05.	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Cyclooctane; C ₈ H ₁₆ ; [292-64-8]	Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr.		
(-, 2	J. Chem. Eng. Data <u>1987</u> , 32, 60-62.		
VARIABLES:	PREPARED BY:		
T/K = 299	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/° C	x ₁		
26.0 0.9804	0.01956		
AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.		
Concentrations determined spectrophoto- metrically at 372 nm.	ESTIMATED ERRORS:		
	T/K: ± 0.05. x ₁ : ± 1 % (relative error).		

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: \pm 0.05. x_1 : \pm 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) t-Butylcyclohexane; C ₁₀ H ₂₀ ; [3178-22-1]	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*₁

26.0 0.9841

x₂

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: \pm 0.05. x_1 : \pm 1 % (relative error).

266			
COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Benzene; C ₆ H ₆ ; [71-43-2] VARIABLES: T/K = 299		ORIGINAL MEASUREMENTS: Judy, C.L.; Pontikos, N.M.; Acree, W.E., Jr. Phys. Chem. Liq. 1987, 16, 179-187. PREPARED BY: W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/° C	* ₂	<i>x</i> ₁	
26.0	0.9368	0.06316	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solve glass bottles and allow for several days at containment of equilibrated solutions transcoarse filter into tar	wed to equilibrate nstant temperature. ium verified by s. Aliquots of sat- ferred through a	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Benzene; C ₆ H ₆ ; [71-43-2]			McLaughl	McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1959, 863-867.		
			J. Chem.			
VARIABLES:			PREPARED 1	BY:		
Temperature		W.E. Acr	ee, Jr.			
EXPERIMENTAL '	VALUES		l			
T/K	<i>x</i> ₂	<i>*</i> 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.

flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

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 alu-mina column with benzene as eluant.
- (2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

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

	26	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259. PREPARED BY:	
(2) Methylbenzene; C ₇ H ₈ ; [108-88-3]		
VARIABLES:		
T/K = 293	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/° C x ₂	× 1	
20.0 0.9433	0.0567	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature.	(1) 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	
Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained	as received.	
after solvent had evaporated.	ESTIMATED ERRORS:	
	T/K: precision \pm 0.05. x ₁ : \pm 3 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Methylbenzene; C ₇ H ₈ ; [108-	Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. 1994, 33, 1355-1362.
VARIABLES:	PREPARED BY:
T/K = Circa 294 (Ambient Room	W.E. Acree, Jr.
EXPERIMENTAL VALUES	•
t/° C x	x 1
21.0 0	335 0.0665
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Ultraviolet/visible spectropho and centrifugal automatic part	

yzer.

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. subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

- received from manufacturer.
- (2) ACS Grade, 99+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

ESTIMATED ERRORS:

T/K: \pm 2 (Compiler). x_1 : \pm 1.5 % (relative error).

268			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00- (2) Methylbenzene; C ₇ H ₈ ; [10		Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press. PREPARED BY: W.E. Acree, Jr. and J.R. Powell	
' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' '	•		
VARIABLES:			
T/K = 299			
EXPERIMENTAL VALUES			
t/° C	x ₂	x ₁	
26.0	0.9322	0.06785	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, thermometer, and an ultravi spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
Concentrations determined s metrically at 372 nm.	pectrophoto-	ESTIMATED ERRORS:	
		$T/K: \pm 0.05.$ $x_1: \pm 2.5 \%$ (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,2-Dimethylbenzene; C ₈ H ₁₀ ; [95-47-6]	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	× ₁	
26.0 0.9239	0.07611	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 98+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
Concentrations determined spectrophotometrically at 372 nm.	ESTIMATED ERRORS:	
	T/K : \pm 0.05. x_1 : \pm 2.5 % (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press. PREPARED BY: W.E. Acree, Jr. and J.R. Powell	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,3-Dimethylbenzene; C ₈ H ₁₀ ; [108-38-3]		
T/K = 299		
EIPERIMENTAL VALUES		
t/° C	× ₁	
26.0 0.9295	0.07055	
AUXILIAR	Y INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
Concentrations determined spectrophotometrically at 372 nm.	ESTIMATED ERRORS:	
	T/K : \pm 0.05. x_1 : \pm 2.5 % (relative error).	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,4-Dimethylbenzene; C ₈ H ₁₀ ; [106-42-3]		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: \pm 0.05. x_1 : \pm 2.5 % (relative error).

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] VARIABLES: Temperature		Kravchenko, V.M.; Pastukhova, I.S. Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669. (English translation) PREPARED BY:				
					W.E. Acree, Jr.	
					EXPERIMENTAL VALUES	
		T/K	<i>x</i> ₂	<i>x</i> 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:

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Miyagishi, S.; Isomi, A.; Iwata, T.; Asakawa, T.; Nishida, M. Bull. Chem. Soc. Japan <u>1985</u> , 58, 3643- 3644.
VARIABLES:	PREPARED BY:
	W.E. Acree, Jr.

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.

AUTILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Differential scanning calorimeter and an (1) Analytical grade, Katayama Chemicals, Japan, was used as received. analytical balance. Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric techniques. (2) Reagent grade, Katayama Chemicals, Japan, was used as received. ESTIMATED ERRORS: T/K: precision \pm 0.3 (Compiler). x_1 : \pm 0.02 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Pyrene; C₁₆H₁₀; [129-00-0] Ethyl ethanoate; C₄H₈O₂; [14] 	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	* 1
26.0 0.9	0.04251
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calc	

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.

- lized 3 times from methanol.
- (2) 99.9 %, Aldrich Chemical Company, was stored over molecular sieves and dis-tilled shortly before use.

ESTIMATED ERRORS:

T/K: \pm 0.05. x_1 : \pm 1.3 % (relative error).

212						
COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Butyl ethanoate; C ₆ H ₁₂ O ₂ ; [123-86-4] VARIABLES: T/K = 299		ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press. PREPARED BY: W.E. Acree, Jr. and J.R. Powell				
				EXPERIMENTAL VALUES		
				t/° C	* ₂	x ₁
26.0	0.9407	0.05932				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCE	DURE	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.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.				
		(2) 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.				
Concentrations determi metrically at 372 nm.	ned spectrophoto-	ESTIMATED ERRORS:				
		T/K : \pm 0.05. x_1 : \pm 2.5 % (relative error).				

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Ethyl butyrate; C ₆ H ₁₂ O ₂ ; [105-54-4]		Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. 1994, 33, 1355-1362.	
VARIABLES:		PREPARED BY:	
T/K = Circa 294 (Ambient Room)		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
40 -	x ₂	x_1	
t/° C	•		

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:

- 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: \pm 2 (Compiler). x_1 : \pm 6.0 % (relative error).

		27	
COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,1-Oxybisbutane; C ₂ H ₁₂ O;		ORIGINAL MEASUREMENTS: Wallach, J.R.; Tucker, S.A.; Oswalt, B.M.; Murral, D.J.; Acree, W.E., Jr.	
			[142-96-1]
VARIABLES: T/K = 299		PREPARED BY: W.E. Acree, Jr.	
			EIPERIMENTAL VALUES
t/° C	x ₂	× ₁	
26.0	0.9702	0.0298	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determine metrically at 372 nm.		ESTIMATED ERRORS:	

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.
Environ. Sci. Technol. 1990, 24, 639-646.
PREPARED BY:
W.E. Acree, Jr.

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:

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

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

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

274	
COMPONENTS:	ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,4-Dioxane; C ₄ H ₈ O ₂ ; [123-91-1]	
<u> </u>	Phys. Chem. Liq., in press.
VARIABLES:	PREPARED BY:
T/K = 299	W.E. Acree, Jr. and J.R. Powell
EIPERIMENTAL VALUES	-
t/° C x ₂	<i>x</i> ₁
26.0 0.9648	0.03520
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.
Concentrations determined spectrophoto- metrically at 372 nm.	ESTIMATED ERRORS:
·	T/K : \pm 0.05. x_1 : \pm 1.3 % (relative error).

COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Tetrachloromethane; CCl ₄ ; [56-23-5] VARIABLES: Temperature		ORIGINAL MEASUREMENTS:			
		McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 2485-2488. PREPARED BY: W.E. Acree, Jr.			
			EXPERIMENTAL VALUES		
			T/K	<i>x</i> ₂	<i>x</i> 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		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		(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.			
noting the temperature trace of solid solute	at which the last	ESTIMATED ERRORS:			
crace or solin solute disappeared.		T/K : precision \pm 0.1. x_1 : \pm 0.0003 (compiler).			

		275			
(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. PREPARED BY:			
			T/K = 299		W.E. Acree, Jr. and J.R. Powell
			EXPERIMENTAL VALUES		
t/° C	x ₂	<i>x</i> ₁			
26.0	0.9577	0.04229			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric		(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,2-Dichloroethane; C ₂ H ₄ Cl ₂ ; [107-06-2]	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

t/° C

x2

26.0

0.9125

x₁ 0.08746

ESTIMATED ERRORS:

T/K: \pm 0.05. x_1 : \pm 1.3 % (relative error).

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

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

flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 372 nm.

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 spectrophoto-metrically 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, anhy-drous, was stored over molecular sieves and distilled shortly before

ESTIMATED ERRORS:

T/K: \pm 0.05. x_1 : \pm 2.5 % (relative error).

276					
COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1-Chlorobutane; C ₄ H ₉ Cl; [109-69-3] VARIABLES: T/K = 299		ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press. PREPARED BY: W.E. Acree, Jr. and J.R. Powell			
			EXPERIMENTAL VALUES		
			t/° C	<i>x</i> ₂	<i>x</i> ₁
			26.0	0.9391	0.06094
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.			
Concentrations determine metrically at 372 nm.	ned spectrophoto-	ESTIMATED ERRORS:			

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,4-Dichlorobutane; C ₄ H ₈ Cl 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:		PREPARED BY:
			<i>T</i> /K = 299		W.E. Acree, Jr.
EXPERIMENTAL VALUES					
t/° C	* ₂	<i>x</i> ₁			
26.0	0.8903	0.1097			
	AUXILI	TARY 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:

T/K: \pm 0.05. x_1 : \pm 2.5 % (relative error).

- (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 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:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (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.

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.

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. (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). x1: ± 0.02 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Methanol; CH ₄ O; [67-56-1]	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

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

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: \pm 1. c₁: \pm 5% (relative error; compiler).

278		
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Methanol; CH ₄ O; [67-56-1] VARIABLES:		ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press. PREPARED BY:
EXPERIMENTAL VALUES		•
t/° C	x ₂	<i>x</i> ₁
26.0	0.9985	0.00149
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEI	URE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.
Concentrations determine metrically at 372 nm.		ESTIMATED ERRORS:
		T/K: ± 0.05. x ₁ : ± 1.3 % (relative error).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Ethanol; C ₂ H ₆ O; [64-17-5]		ORIGINAL MEASUREMENTS:	
		Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259.	
			VARIABLES:
T/K = 293		W.E. Acree, Jr.	
EIPERIMENTAL VALUES		!	
t/° C	x ₂	× 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 \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

		27			
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Ethanol; C ₂ H ₆ O; [64-17-5]		ORIGINAL MEASUREMENTS: 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	0.9968	0.00317			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.		(2) Absolute, Aaper Alcohol and Chemical Company, Shelbyville, Kentucky, USA, was stored over molecular sieves and distilled shortly before use.			
		ESTIMATED ERRORS:			
		T/K : \pm 0.05. x_1 : \pm 1.3 % (relative error).			

COMPONER	NTS:		ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1-Propanol; C ₃ H ₈ O; [71-23-8]		29-00-0]	Zvaigzne, A.I.; Acree, W.E., Jr.
			J. Chem. Eng. Data <u>1993</u> , 38, 393-395.
VARIABLES:			PREPARED BY:
T/K = 2	299		W.E. Acree, Jr.
EXPERIME	NTAL VALUES		
	t/° C	* ₂	× ₁
	26.0	0.9957	0.00426
		AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE		EDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.			(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.		owed to equilibrate onstant temperature. rium verified by tas. Aliquots of satserred through a red volumetric	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
		ined spectrophoto-	ESTIMATED ERRORS:
			T/K: ± 0.05. x ₁ : ± 1.5 % (relative error).

urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

280 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Zvaigzne, A.I.; Acree, W.E., Jr. (2) 2-Propanol; C₃H₈O; [67-63-0] J. Chem. Eng. Data 1993, 38, 393-395. PREPARED BY: VARIABLES: T/K = 299W.E. Acree, Jr. EXPERIMENTAL VALUES t/º C x₂ x₁ 26.0 0.9971 0.00290 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 3 times from absolute ethanol. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by (2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. repetitive measurements. Aliquots of sat-

ESTIMATED ERRORS:

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

COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1-Butanol; C ₄ H ₁₀ O; [71-36-3] VARIABLES: T/K = 299 EXPERIMENTAL VALUES		ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press. PREPARED BY: W.E. Acree, Jr. and J.R. Powell
t/° C	x 2	x ₁
26.0	0.9938	0.00622
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bethermometer, and an ule spectrophotometer. Excess solute and solve glass bottles and alloe for several days at constant and the several days are several days.	ent placed in amber wed to equilibrate nstant temperature. ium verified by s. Aliquots of satferred through a ed volumetric luted with methanol.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol. (2) 99.8 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.
Concentrations determine metrically at 372 nm.	ned spectrophoto-	ESTIMATED ERRORS: T/K: ± 0.05. x ₁ : ± 1.3 % (relative error).

	28
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr.
(2) 2-Butanol; C ₄ H ₁₀ O; [15892-23-6]	Phys. Chem. Liq., in press.
variables:	PREPARED BY:
T/K = 299	W.E. Acree, Jr. and J.R. Powell
EIPERIMENTAL VALUES	•
t/° C x ₂	x ₁
26.0 0.9957	0.00433
AUXILIAR	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Aldrich Chemical Company, anhy- drous, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spectrophoto- metrically at 372 nm.	ESTIMATED ERRORS:
	T/K : ± 0.05 . x_1 : ± 1.3 % (relative error).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1-Pentanol; C ₅ H ₁₂ O; [71-41-0]		ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press.
T/K = 299		W.E. Acree, Jr. and J.R. Powell
EXPERIMENTAL VALUES		
t/° C	*2	x ₁
26.0	0.9907	0.00926
	AUXILI	MARY INFORMATION
METHOD: APPARATUS/PROCE	DURE	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 372 nm.

- (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: \pm 0.05. x_1 : \pm 1.3 % (relative error).

COMPONENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. (2) 2-Methyl-1-propanol; C₄H₁₀O; Phys. Chem. Liq., in press. VARIABLES: PREPARED BY: T/K = 299 W.E. Acree, Jr. and J.R. Powell EXPERIMENTAL VALUES

t/º C

 $\boldsymbol{x_2}$

26.0

0.9968

X₁

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: \pm 0.05. x_1 : \pm 1.3 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 3-Methyl-1-butanol; C ₅ H ₁₂ O; [123-51-3]	Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Lig., in press.
VARIABLES:	PREPARED BY:
T/K = 299	W.E. Acree, Jr. and J.R. Powell

EXPERIMENTAL VALUES

t/º C

x₂

26.0

0.9945

x1

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: \pm 0.05. x_1 : \pm 1.3 % (relative error).

ORIGINAL MEASUREMENTS: COMPONENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. (1) Pyrene; C₁₆H₁₀; [129-00-0] (2) 1-Octanol; C₈H₁₈O; [111-87-5] Phys. Chem. Liq., in press. PREPARED BY: VARIABLES: W.E. Acree, Jr. and J.R. Powell T/K = 299EXPERIMENTAL VALUES t/° C x_2 x_1 0.9790 0.02097 26.0 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 3 times from methanol. spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate (2) 99+ %, Aldrich Chemical Company, anhy-drous, was stored over molecular sieves and distilled shortly before for several days at constant temperature. Attainment of equilibrium verified by use. repetitive measurements. Aliquots of saturated solutions transferred through a

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D. Environ. Sci. Technol. 1985, 19, 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.

ESTIMATED ERRORS: T/K: \pm 0.05.

 x_1 : \pm 1.3 % (relative error).

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.

coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 372 nm.

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:

- 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: \pm 0.1 (compiler). c_1 : ± 3 % (relative error; compiler).

284		
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Cyclopentanol; C ₅ H ₁₀ O; [96-41-3]		ORIGINAL MEASUREMENTS: Powell, J.R.; Voisinet, D.; Salazar, A.; Acree, W.E., Jr. Phys. Chem. Liq., in press.
T/K ≠ 299		
EXPERIMENTAL VALUES		-1
t/° C	x ₂	x ₁
26.0	0.9901	0.00994
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEI	URE	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.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.
		(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.
Concentrations determine metrically at 372 nm.	ed spectrophoto-	ESTIMATED ERRORS:
		T/K : \pm 0.05. x_1 : \pm 1.3 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1-Hydroxy-2-methylbenzene; C ₇ H ₈ O; [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.
	•

t/ºC

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

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:

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

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

	289
COMPONENTS:	ORIGINAL MEASUREMENTS: Krezewki, R.; Smutek, M. Collection Czech. Chem. Commun. 1967, 32, 1258-1259. PREPARED BY: W.E. Acree, Jr.
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	
(2) 2-Propanone; C ₃ H ₆ O; [67-64-1]	
VARIABLES:	
T/K = 293	
EIPERIMENTAL VALUES	·
t/° C	x ₁
20.0 0.9716	0.0284
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	 95 % initial purity, source not given, was recrystallized several times from toluene and ethanol to give a melting temperature of 150.5-150.9 °C. Commercial sample, purity and source not specified, was dehydrated and distilled before use.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:
	T/K: precision \pm 0.05. x ₁ : \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 2-Propanone; C ₃ H ₆ O; [67-64-1]	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	
EIPERIMENTAL VALUES		
t/° C	× ₁	
26.0 0.9639	0.03612	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
Concentrations determined spectrophoto- metrically at 372 nm.	ESTIMATED ERRORS:	
	T/K : \pm 0.05. x_1 : \pm 1.3 % (relative error).	

286 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Krezewki, R.; Smutek, M. (2) Pyridine; C₅H₅N; [110-86-1] Collection Czech. Chem. Commun. 1967, 32, 1258-1259. VARIABLES: PREPARED BY: T/K = 293W.E. Acree, Jr. EXPERIMENTAL VALUES t/° C x₂ X₁ 0.0873 20.0 0.9127 **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.,
- (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 \pm 0.05. x_1 : \pm 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Dimethyl sulfoxide; C ₂ H ₆ OS; [67-68-5]	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 c₁/(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:

- Purity not given, commercial sample of unspecified source, was used as received.
- (2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Carre, O.R.; Phillips, D.J.; Brennecke, J.F. Ind. Eng. Chem. Res. 1994, 33, 1355-1362.
VARIABLES:	PREPARED BY:
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.

t/° C

x₂

21.0

0.9943

*x*₁

0.00574

AUXILIARY INFORMATION

METBOD: 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).

ORIGINAL MEASUREMENTS: COMPONENTS: Shinomiya, C. (1) Pyrene; C₁₆H₁₀; [129-00-0] (2) 1,3-Dinitrobenzene; $C_6H_4N_2O_4$; [99-65-0] J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K T/K x, x₁ x₁ x₂ 0.446 1.000 0.000 365.0 0.554 363.2 358.2 0.913 0.087 365.7 0.499 0.501 0.504 354.2 0.854 0.146 366.0 0.496 357.2 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 0.621 0.379 384.2 0.341 0.659 362.2 363.7 0.586 0.414 395.7 0.277 0.723 1.000 364.7 0.563 0.437 423.2 0.000

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 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). x₁: ± 0.002 (Compiler).

COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,4-Dinitrobenzene; C ₆ H ₄ N ₂ O ₄ ; [100-25-4] VARIABLES: Temperature		ORIGINAL MEASUREMENTS:			
		Shinomiya, C.			
		J. Chem. Soc. Japan <u>1940</u> , 15, 259-270.			
		PREPARED BY:			
		W.E. Acree, Jr.			
EXPERIMENTAL	VALUES				
T/K	<i>x</i> ₂	×1	T/K	x ₂	<i>x</i> 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	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 \pm 0.2 (Compiler). x ₁ : \pm 0.002 (Compiler).	

ORIGINAL MEASUREMENTS: COMPONENTS: Shinomiya, C. (1) Pyrene; C₁₆H₁₀; [129-00-0] (2) 1,3,5-Trinitrobenzene; C₆H₃N₃O₆; [99-35-4] J. Chem. Soc. Japan 1940, 15, 259-270. VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K Solid Phase x₁ **x**₂ 1.000 0.000 396.2 (2) 1:1 Compound 420.2 0.950 0.050 0.828 0.172 1:1 Compound 478.2 0.826 0.174 1:1 Compound 478.2 500.2 0.740 0.260 1:1 Commpound 0.627 0.373 1:1 Compound 514.7 518.7 0.514 0.486 1:1 Compound 517.2 0.447 0.553 1:1 Compound 0.321 0.679 1:1 Compound 508.7 0.778 0.222 1:1 Compound 482.5 0.160 0.840 1:1 Compound 466.7 0.875 1:1 Compound 439.2 0.125 423.2 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 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). x₁: ± 0.002 (Compiler).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 1,2,3,5-Tetranitrobenzene; C ₆ H ₂ N ₄ O ₈ ; [3698-53-1]		ORIGINAL MEASUREMENTS:		
		Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270.		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
<i>T</i> /K	<i>x</i> ₂	<i>x</i> 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	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).	

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Shinomiya, C. (2) 2,4-Dinitromethylbenzene; $C_7H_6N_2O_4$; [121-14-2] J. Chem. Soc. Japan 1940, 15, 259-270. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K Solid Phase x_1 ×2 344.2 1.000 0.000 (2) 0.823 0.178 (2) 333.7 337.2 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 0.481 1:1 Compound 365.2 0.519 365.7 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.

METHOD: APPARATUS/PROCEDURE 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). x₁: ± 0.002 (Compiler).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 2,4-Dinitrophenol; C ₆ H ₄ N ₂ O ₅ ; [51-28-5] VARIABLES: Temperature		ORIGINAL MEASUREMENTS: Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: W.E. Acree, Jr.						
					EXPERIMENTAL VALUES			
					T/K	x ₂	<i>×</i> 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		
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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).		

COMPONENTS: ORIGINAL MEASUREMENTS: Shinomiya, C. (1) Pyrene; C₁₆H₁₀; [129-00-0] (2) 2,4,6-Trinitromethylbenzene; C₇H₅N₃O₆; [118-96-7] J. Chem. Soc. Japan 1940, 15, 259-270. **VARIABLES:** PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K x_1 \mathbf{x}_{2} 354.7 1.000 0.000 (2) 354.2 0.056 0.944 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 0.431 436.7 0.569 1:1 Compound 427.2 0.315 0.685 1:1 Compound 0.239 0.761 1:1 Compound 415.7 405.2 0.156 0.844 (2) 0.971 421.2 0.029 (2) 0.000 1.000 423.2 (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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).	

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 2,4,6-Trinitromethoxybenzene; C ₇ H ₅ N ₃ O ₇ ; [606-35-9] VARIABLES: Temperature		ORIGINAL MEASUREMENTS: Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: W.E. Acree, Jr.						
					EIPERIMENTAL VALUES			¥
					T/K	x ₂	<i>*</i> 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).			

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Shinomiya, C. (2) 2,4,6-Trinitroaniline; C₆H₄N₃O₆; [489-98-5] J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY: VARIABLES: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K X₁ x₂ 0.000 461.7 1.000 (2) 468.7 0.166 1:1 Compound 0.834 0.731 1:1 Compound 486.7 0.269 0.614 0.386 1:1 Compound 504.2 509.2 0.503 0.497 1:1 Compound 0.480 0.520 1:1 Compound 508.7 505.5 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 0.118 447.2 0.882 1:1 Compound 442.2 1:1 Compound 0.085 0.915 0.947 418.2 0.053 (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 SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source were not No experimental details given in paper. specified in paper. (2) Purity and chemical source were not specified in paper. ESTIMATED ERRORS: T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 2-Chloro-1,3,5-trinitrobenzene; C ₆ H ₂ ClN ₃ O ₆ ; [88-88-0]		ORIGINAL MEASUREMENTS:		
		Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270.		
				VARIABLES:
Temperature		W.E. Acree, Jr.		
EIPERINENTAL 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Krajewska, A.; Wasilewska, K.
(2) 2-Chloro-1,3,5-trinitrobenzene; C ₆ H ₂ C1N ₃ O ₆ ; [88-88-0]	Thermochim. Acta <u>1981</u> , 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 SOURCE AND PURITY OF MATERIALS: Differential scanning calorimeter and thermostated light microscope. (1) Purity and chemical source were not specified in paper. Binary mixtures were prepared by weight. Melting point temperatures and phase diagram determined using differential scanning calorimetric and microscopic (2) Purity and chemical source were not specified in paper. techniques. ESTIMATED ERRORS: T/K: precision \pm 0.1 (Compiler). x_1 : \pm 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Bando, M.; Matsunaga, Y.
(2) 2-Chloro-1,3,5-trinitrobenzene; C ₆ H ₂ ClN ₃ O ₆ ; [88-88-0]	Bull. Chem. Soc. Japan <u>1976</u> , 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 SOURCE AND PURITY OF MATERIALS: Differential scanning calorimeter. (1) Purity and chemical source were not specified in paper. Binary mixtures were prepared by weight. Melting points and transition tempera-(2) Purity and chemical source were not tures determined using a differential specified in paper. scanning calorimeter An experimental phase diagram is given in the original paper. ESTIMATED ERRORS: T/K: precision \pm 0.1 (Compiler). x_1 : \pm 0.002 (Compiler).

(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) 3-Methyl-2,4,6-trinitrophenol; C ₇ H ₅ N ₃ O ₇ ; [602-99-3]		ORIGINAL ME	ORIGINAL MEASUREMENTS: Shinomiya, C. J. Chem. Soc. Japan 1940, 15, 259-270. PREPARED BY:		
		Shinomiya,			
		J. Chem. S			
VARIABLES:	VARIABLES:				
Temperature		W.E. Acree	W.E. Acree, Jr.		
EIPERIMENTAL VAI	UES	<u></u>			
T/K	x ₂	<i>*</i> 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 reddishbrown 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

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). x₁: ± 0.002 (Compiler).

COMPONENTS:

- (1) Pyrene; C₁₆H₁₀; [129-00-0]
- (2) n-Hexane; C₆H₁₄; [110-54-3]
- (3) 1-Propanol; C₃H₈O; [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

(e)		
x3 ^(s)	<i>x</i> ₃	х 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; $x_1\colon$ mole fraction solubility of the solute; $x_3\colon$ 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: \pm 0.05. $x_3^{(s)}$: \pm 0.0001. x_1 : \pm 1.5 % (relative error).

COMPONENTS:

- (1) Pyrene; C₁₆H₁₀; [129-00-0]
- (2) n-Heptane; C₇H₁₆; [142-82-5]
- (3) 1-Propanol; C₃H₈O; [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

+	_	26	Λ	٥٥

x3 ^(s)	x ₃	<i>*</i> 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:

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

COMPONENTS: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) n-Octane; C ₈ H ₁₈ ; [111-65-9] (3) 1-Propanol; C ₃ H ₈ O; [71-23-8] VARIABLES: T/K = 299, Solvent composition		ORIGINAL MEASUREMENTS:
		Zvaigzne, A.I.; Acree, W.E., Jr.
		J. Chem. Eng. Data 1993, 38, 393-395.
		PREPARED BY:
		W.E. Acree, Jr. and A.I. Zvaigzne
EXPERIMENTAL VALU	ES ^a	
*3 ^(s)	<i>x</i> ₃	×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

METHOD: APPARATUS/PROCEDURE

the ternary solution.

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

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equili-brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

- (1) 99 %, Aldrich Chemical Company, Milwau-kee, 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: \pm 0.05. $x_3^{(s)}$: \pm 0.0001. x_1 : \pm 1.5 % (relative error).

COMPONENTS:

- (1) Pyrene; C₁₆H₁₀; [129-00-0]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]
- (3) 1-Propanol; C₃H₈O; [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

t =	26.0	°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

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

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

304 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Zvaigzne, A.I.; Acree, W.E., Jr. J. Chem. Eng. Data 1993, 38, 393-395. (2) Methylcyclohexane; C₇H₁₄; [108-87-2] (3) i-Propanol; C₃H₈O; [71-23-8] PREPARED BY: VARIABLES: W.E. Acree, Jr. and A.I. Zvaigzne T/K = 299, Solvent composition EXPERIMENTAL VALUES^a $t = 26.0 \, {}^{\circ}\text{C}$ x3(8) x_1 x_3 0.0000 0.01292 0.0000 0.1734 0.1711 0.01336 0.2997 0.2959 0.01271

 a $x_{x}^{(s)}$: 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

0.01045

0.00921

0.00798

0.00599

0.00499

0.00426

METHOD: APPARATUS/PROCEDURE

0.5273

0.6238

0.7164

0.8672 0.9384

1.0000

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

0.5218

0.6181

0.7107

0.8620

0.9337

0.9957

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, Milwau-kee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical

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

ESTIMATED ERRORS:

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

COMPONENTS:

- (1) Pyrene; C₁₆H₁₀; [129-00-0]
- (2) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]
- (3) 1-Propanol; C₃H₈O; [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

x3 ^(s)	<i>x</i> 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

 $[^]a$ $x_3^{(s)}\colon$ initial mole fraction of binary solvent mixture; $x_1\colon$ mole fraction solubility of the solute; $x_3\colon$ 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 spectrophoto-metrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

- (1) 99 %, Aldrich Chemical Company, Milwau-kee, 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:

 $x_3^{(s)}$: ± 0.05 . $x_3^{(s)}$: ± 0.0001 . x_1 : ± 1.5 % (relative error).

306		
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H	₁₀ ; [129-00-0]	Zvaigzne, A.I.; Acree, W.E., Jr. J. Chem. Eng. Data 1993, 38, 393-395.
(2) n-Hexane; C ₆	H ₁₄ ; [110-54-3]	
(3) 2-Propanol;	C ₃ H ₈ O; [67-63-0]	
VARIABLES:		PREPARED BY:
T/K = 299, Solve	ent composition	W.E. Acree, Jr. and A.I. Zvaigzne
EXPERIMENTAL VALUE t = 26.0 °C	ues ^a	
x3 ⁽⁸⁾	<i>x</i> ₃	<i>x</i> ₁
0.0000	0.0000	0.00857
0 1676	0 1661	0.00067

x3 ⁽⁸⁾	x ₃	<i>x</i> 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; $x_1\colon$ mole fraction solubility of the solute; $x_3\colon$ mole fraction of component 3 in the ternary solution.

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:

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

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Zvaigzne, A.I.; Acree, W.E., Jr. (2) n-Heptane; C₇H₁₆; [142-82-5] J. Chem. Eng. Data 1993, 38, 393-395. (3) 2-Propanol; C₃H₈O; [67-63-0] VARIABLES: PREPARED BY: T/K = 299, Solvent composition W.E. Acree, Jr. and A.I. Zvaigzne EXPERIMENTAL VALUES^a $t = 26.0 \, ^{\circ}C$ x3⁽⁸⁾ x, x_3 0.0000 0.0000 0.01102 0.1872 0.1851 0.01117 0.01029 0.3336 0.3302

0.00830

0.00724

0.00618

0.00430

0.00367

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.

0.5515

0.6511

0.7390

0.8852

0.9356

0.9971

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

0.5561

0.6558

0.7436

0.8890

0.9390

1,0000

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) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H	₁₀ ; [129-00-0]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Octane; Cg	H ₁₈ ; [111-65-9]	J. Chem. Eng. Data <u>1993</u> , 38, 393-395
(3) 2-Propanol;	c ₃ H ₈ O; [67-63-0]	
/ARIABLES:		PREPARED BY:
T/K = 299, Solve	ent composition	W.E. Acree, Jr. and A.I. Zvaigzne
EXPERIMENTAL VALUE t = 26.0 °C	TES ⁸	
*3 ^(s)	<i>x</i> 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

METEOD: 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 spectrophoto-metrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

- 99 %, Aldrich Chemical Company, Milwau-kee, 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:

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

COMPONENTS:

- (1) Pyrene; C₁₆H₁₀; [129-00-0]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]
- (3) 2-Propanol; C₃H₈O; [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

t	=	26.	0	°C

x3 ^(s)	<i>x</i> ₃	<i>x</i> 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

 $[^]a$ $x_3^{(s)}\colon$ initial mole fraction of binary solvent mixture; $x_1\colon$ mole fraction solubility of the solute; $x_3\colon$ mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METEOD: 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:

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

310		
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁	₁₀ ; [129-00-0]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2] (3) 2-Propanol; C ₃ H ₈ O; [67-63-0]		J. Chem. Eng. Data <u>1993</u> , 38, 393-395.
VARIABLES:		PREPARED BY:
T/K = 299, Solve	ent composition	W.E. Acree, Jr. and A.I. Zvaigzne
EXPERIMENTAL VALUE t = 26.0 °C	JES ^a	
x3 ^(s)	x ₃	× 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

0.00469

0.00374

0.00290

AUXILIARY INFORMATION

METEOD: APPARATUS/PROCEDURE

0.8660

0.9336

1,0000

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

0.8619

0.9301

0.9971

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 spectrophoto-metrically at 372 nm.

SOURCE AND PURITY OF MATERIALS:

- (1) 99 %, Aldrich Chemical Company, Milwau-kee, 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: \pm 0.05. $x_3^{(6)}$: \pm 0.0001. $x_1^{(6)}$: \pm 1.5 % (relative error).

 $[^]a$ $x_3^{(s)};$ initial mole fraction of binary solvent mixture; $x_1\colon$ mole fraction solubility of the solute; $x_3\colon$ mole fraction of component 3 in the ternary solution.

COMPONENTS:

- (1) Pyrene; C₁₆H₁₀; [129-00-0]
- (2) 2,2,4-Trimethylpentane; C_8H_{18} ;
- [540-84-1] (3) 2-Propanol; C₃H₈O; [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

) ⁰(

x3 ^(s)	<i>x</i> 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.

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, Milwau-kee, 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: \pm 0.05. $x_3^{(s)}$: \pm 0.0001. x_1 : \pm 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. <u>Ketones</u>
- I. Miscellaneous Pure Solvents

phenothiazine phenoxanthiin phenoxazine

J. Binary Solvent Mixtures

313 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Thianthrene; C₁₂H₈S₂; [92-85-3] Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, (2) n-Hexane; C₆H₁₆; [110-54-3] Phys. Chem. Liq. 1990, 21, 45-49. VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/° C **x**2 x₁ 25.0 0.9968 0.00320 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric (1) 99 %, Aldrich Chemical Company, thermometer, and an ultraviolet/visible spectrophotometer. Milwaukee, Wisconsin, USA, recrystal-lized 3 times from absolute ethanol. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate (2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and disfor several days at constant temperature. tilled shortly before use. 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) Thianthrene; C ₁₂ H ₈ S ₂ ; [92-85-3] (2) n-Heptane; C ₇ H ₁₆ ; [142-82-5]		ORIGINAL MEASUREMENTS: Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I. Phys. Chem. Liq. 1990, 21, 45-49.	
EXPERIMENTAL VALUES			
t/° C	x ₂	x ₁	
25.0	0.9965	0.00346	

ESTIMATED ERRORS:

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

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: \pm 0.05. x_1 : ± 1 % (relative error).

314			
(1) Thianthrene; C ₁₂ H ₈ S ₂ ; [92-85-3] (2) n-Octane; C ₈ H ₁₈ ; [111-65-9]		ORIGINAL MEASUREMENTS: Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.	
VARIABLES:			
T/K = 298			
EXPERIMENTAL VALUES			
t/° C	x ₂	<i>x</i> ₁	
25.0	0.9961	0.00392	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determine metrically at 255 nm.	ed spectrophoto-	ESTIMATED ERRORS:	
		T/K : ± 0.05 . x_1 : ± 1 % (relative error).	

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Thianthrene; C ₁₂ F	• •	Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.				
(2) Cyclohexane; C ₆ H	₁₂ ; [110-82-7]	Phys. Chem. Liq. 1990, 21, 45-49.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES		•				
t/° C	x ₂	<i>x</i> ₁				
25.0	0.9941	0.00587				
	, AUXILIARY	INFORMATION				
METHOD: APPARATUS/PRO	CEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature thermometer, and an spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.				
glass bottles and all for several days at a Attainment of equilibrepetitive measurement urated solutions tra- coarse filter into to	constant temperature. brium verified by nts. Aliquots of sat- nsferred through a	(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.				
Concentrations determine metrically at 255 nm.		ESTIMATED ERRORS:				
		T/K : ± 0.05 . x_1 : ± 1 % (relative error).				

		31
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Thianthrene; C ₁₂ H ₈ S ₂ ;		Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.
(2) Methylcyclohexane; C [108-87-2]	7 ^H 14;	Phys. Chem. Liq. 1990, 21, 45-49.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES ^a		
t/° C	<i>x</i> ₂	<i>x</i> ₁
25.0	0.9937	0.00631
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDU	RE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bat thermometer, and an ultra spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.
Excess solute and solvenglass bottles and allower for several days at constatainment of equilibrium repetitive measurements. urated solutions transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks, weighed and diluter transfer coarse filter into tared flasks.	d to equilibrate tant temperature. m verified by Aliquots of sat-rred through a volumetric ted with methanol.	(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined metrically at 255 nm.	i spectrophoto-	ESTIMATED ERRORS:

c ₁₂ H ₈ s ₂ ; [92-85-3]	Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, A.I.				
C ₈ H ₁₆ ; [292-64-8]					
	PREPARED BY:				
	W.E. Acree, Jr.				
JES ^a					
x ₂	<i>x</i> ₁				
0.9877	0.01232				
_	-				

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:

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

- (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: \pm 0.05. x_1 : \pm 1 % (relative error).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Thianthrene; C₁₂H₈S₂; [92-85-3] Acree, W.E., Jr.; Tucker, S.A.; Zvaigzne, (2) 2,2,4-Trimethylpentane; CgH18; [540-84-1] Phys. Chem. Liq. 1990, 21, 45-49. PREPARED BY: VARIABLES: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES⁸ t/º C x, x, 0.9973 25.0 0.00273 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 3 times from absolute ethanol. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by (2) HPLC Grade, 99.7 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 255 nm. ESTIMATED ERRORS: T/K: \pm 0.05. x_1 : \pm 1 % (relative error).

COMPONENTS: ORIGINAL MEASUREMENTS: Mayer, M.M.; Howell, W.J.; Tomasko, D.L.; (1) Thianthrene; C₁₂H₈S₂; [92-85-3] Eckert, C.A. J. Chem. Eng. Data 1990, 35, 446-449. (2) Phenanthrene; C14H10; [85-01-8] VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES Solid Phase T/K \mathbf{x}_{2} x₁ 0.00 1.00 372 (2) 0.95 0.05 (2) 369 0.90 0.10 (2) 365 0.85 0.15 (2) 361 0.80 0.20 357 (2) 0.75 0.25 356 (1) 0.70 0.30 (1) 362 370 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) 0.40 0.60 400 (1) 0.35 0.65 405 (1) 409 0.30 0.70 (1) 0.25 0.75 412 (1) 0.20 0.80 416 (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

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:

- 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 \pm 0.5. x_1 : \pm 0.005 (Compiler).

components:		ORIGINAL MEASUREMENTS:				
(1) Thianthrene; C ₁₂ H ₈	s ₂ ; [92-85-3]	Cullinane, N.M.; Rees, W.T.				
(2) Phenothiazine; C ₁₂ H ₉ NS; [92-84-2]		Trans. Faraday Soc. <u>1940</u> , 36, 506-514.				
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL VALUES ⁸						
$ au_{\sf in}/{\sf K}$	T _{fin} /K	*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 $x_2 = 1.00$. $T_{\rm in}$ refers to the temperature at which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported tempera-

METHOD: APPARATUS/PROCEDURE

tures verified by repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

- 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 \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).

					<u>ی</u>		
COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Thianthro	ene; C ₁₂ H ₈ S ₂ ;	[92-85-3]	Cullinane, N.M	.; Rees, W.T	•		
(2) Phenoxan	thiin; C ₁₂ H ₈ O	s; [262-20-4]	Trans. Faraday	Soc. 1940,	36, 506-514.		
VARIABLES:	ARIABLES:						
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL V	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		
		AUXILIAR	(INFORMATION				
METHOD: APPARI	ATUS/PROCEDU	RE	SOURCE AND PURITY OF MATERIALS:				
tubes. Tempe with ample to	erature was s Lme given for	small capillary slowly varied e equilibration.	(1) Purity and chemical source not speci- fied, was purified by sublimation and recrystallized from acetone.				
Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.		(2) Synthesized by authors, was purified by sublimation and recrystallized from alcohol.					
			ESTIMATED ERRORS	5:			
			T/K: precision \pm 0.2 (Compiler). x_1 : \pm 0.002 (Compiler).				

Components:			ORIGINAL MEASUREMENTS: Cullinane, N.M.; Rees, W.T. Trans. Faraday Soc. 1940, 36, 506-514. PREPARED BY:				
(1) Thianthr	ene; C ₁₂ H ₈ S ₂ ;	[92-85-3]					
(2) Phenoxaz	ine; C ₁₂ H ₉ NO;	[135-67-1]					
/ARIABLES:							
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL	VALUES		!				
T/K	x ₂	x ₁	T/K	x ₂	<i>x</i> 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					

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:

- 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 \pm 0.2 (Compiler). x_1 : \pm 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. <u>Ketones</u>
- I. Miscellaneous Pure Solvents

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:			ORIGINAL N	MEASUREMENTS:			
	hene; C ₁₃ H ₁₀ S; ane; C ₆ H ₁₂ ; [1		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.				
(2) Cyclonesi	ane, 6,12, 1-	.10-02-7]	J. Soluti	ion Chem. 19	<u>88</u> , 16, 519-534.		
VARIABLES:			PREPARED BY:				
Temperature			W.E. Acre	e, Jr.			
EXPERIMENTAL V	VALUES						
T/K	x ₂	<i>x</i> ₁	T/K	x 2	<i>x</i> 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	ī			
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
thermometer.	Constant temperature bath and a precision thermometer.			(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual					cal		
noting the te	emperature at	which the last	ESTIMATED	ERRORS:			
01000 01 0011	,	-pp	T/K : precision \pm 0.1. x_1 : \pm 0.0003.				

(1) Thioxanthene; C ₁₃ H ₁₀ S; [261-31-4] (2) Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8]			ORIGINAL ME	ORIGINAL MEASUREMENTS:				
			Coon, J.E.	Coon, J.E.; Auwaerter, J.E.; Mc				
			Fluid Phase	Fluid Phase Equilibr. 1989, 44, 305-345				
VARIABLES:			PREPARED BY	}				
Temperature			W.E. Acree,	Jr.				
EXPERIMENTAL \	ALUES							
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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						
	0.8971	0.1029						

METEOD: 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:

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Thioxanthene; C ₁₃ H ₁₀ S; [261-31-4] (2) Benzene; C ₆ H ₆ ; [71-43-2]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. 1988, 16, 519-534.					
							VARIABLES:
Temperature			W.E. Acre	ee, Jr.			
EXPERIMENTAL V	VALUES		1				
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	ī			
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
thermometer.	Constant temperature bath and a precision thermometer.			(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.					
noting the te	emperature at	which the last	ESTIMATED	ERRORS:			
		-FF-32021	T/K: pred x ₁ : ± 0.0	ision <u>+</u> 0.1.			

omponents:			ORIGINAL MEASUREMENTS:				
(1) Thioxant	hene; C ₁₃ H ₁₀ S;	[261-31-4]	Coon, J.E.;	Auwaerter,	J.E.; McLaughlin, E		
(2) 1,2,3,4-Tetrahydronaphthalene; C ₁₀ H ₁₂ ; [119-64-2]			Fluid Phase Equilibr. 1989, 44, 305-3				
VARIABLES:			PREPARED BY:				
Temperature			W.E. Acree,	Jr.			
EXPERIMENTAL 1	VALUES						
T/K	<i>x</i> ₂	<i>*</i> 1	T/K	<i>x</i> ₂	<i>x</i> 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					
	0.7956	0.2044					

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:

					02	
COMPONENTS:			ORIGINAL I	MEASUREMENTS:		
(1) Thioxanth			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.			
(2) Pyridine; C ₅ H ₅ N; [110-86-1]		J. Solution Chem. 1988, 16, 519-534.				
VARIABLES:			PREPARED E	BY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL V	VALUES		1			
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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	ī		
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
thermometer.	Constant temperature bath and a precision thermometer.			(1) 99+ %, gift from Dr. E. J. Esienbraun, Oklahoma State University, USA, was recrystallized from toluene.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
	emperature at	which the last	ESTIMATED	ERRORS:		
			T/K: pred x ₁ : ± 0.0	cision <u>+</u> 0.1.		

COMPONENTS:	COMPONENTS:			ORIGINAL MEASUREMENTS:				
	1) Thioxanthene; C ₁₃ H ₁₀ S; [261-31-4] 2) Thiophene; C ₄ H ₄ S; [110-02-1]			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E McLaughlin, E. J. Solution Chem. 1988, 16, 519-534.				
VARIABLES:			PREPARED I	BY:				
Temperature			W.E. Acre	ee, Jr.				
EXPERIMENTAL V	ALUES							
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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						

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:

- 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:

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

<9333

59-430

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Triphenylene; C₁₈H₁₂; [217-59-4] Lissi, E.A.; Abuin, E.B. (2) n-Heptane; C7H16; [142-82-5] Bol. Soc. Chil. Quim. 1981, 26, 19-34. VARIABLES: PREPARED BY: T/K = 293W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(mol dm^{-3})$ t/°C 20.0 0.0056 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, centrifuge, Purity not given, commercial sample of unspecified source, was used as thermometer, and an uv/visible spectrophotometer. received.

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

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

ESTIMATED ERRORS:

T/K: \pm 2. c_1 : unknown.

COMPONENTS:		ORIGINAL	ORIGINAL MEASUREMENTS: McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1959, 863-867.					
(1) Triphenylene; C ₁₈ H ₁₂ ; [217-59-4] (2) Benzene; C ₆ H ₆ ; [71-43-2]								McLaughl:
								J. Chem.
VARIABLES:	1		PREPARED 1	BY:				
Temperature			W.E. Acr	W.E. Acree, Jr.				
EXPERIMENTAL '	VALUES		ļ					
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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						

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:

- 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 \pm 0.1. x_1 : \pm 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] VARIABLES: Temperature		Sturrock, M.G.; Lawe, T.				
		Can. J. Res., Sect. B. <u>1939</u> , 17, 71-74.				
		PREPARED BY:				
		W.E. Acree, Jr.				
EXPERIMENTAL VALUES ^a						
r _{in} /ĸ	T _{fin} /K	x ₂	<i>x</i> 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 $x_1 = 1.00$. $T_{\rm in}$ refers to the temperature which crystallization begins; $T_{\rm fin}$ is the temperature at which crystallization of the solid solution concludes.

METHOD: APPARATUS/PROCEDURE

Melting points and freezing points were obtained by determining temperatures of incipient fusion and complete liquefaction using capillary tube method. Temperature very slowly raised and material observed through a low power microscope.

SOURCE AND PURITY OF MATERIALS:

- (1) Obtained from heavy crude oil, and was recrystallized from alcohol before
- (2) Obtained from heavy crude oil, and was fractionally recrystallized from alcohol before use.

ESTIMATED ERRORS:

T/K: precision \pm 0.5 (Compiler). x_1 : \pm 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. <u>Esters</u>
- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. Alcohols
- H. <u>Ketones</u>
- I. <u>Miscellaneous Pure Solvents</u>

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:			ORIGINAL MEASUREMENTS:										
(1) Xanthene; C ₁₃ H ₁₀ O; [92-83-1]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. 1988, 16, 519-534. PREPARED BY: W.E. Acree, Jr.											
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7] VARIABLES: Temperature													
							EXPERIMENTAL 1	VALUES		<u> </u>			
							T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>*</i> 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			<u> </u>								
		AUXILIARY	INFORMATION	ī									
METHOD: APPARA	ATUS/PROCEDUR	LE .	SOURCE AND	PURITY OF M	ATERIALS:								
thermometer.				(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.									
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.										
noting the to		which the last	ESTIMATED	ERRORS:									
		appoint out	T/K : precision \pm 0.1. x_1 : \pm 0.0003.										

(1) Xanthene; C ₁₃ H ₁₀ O; [92-83-1] (2) Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8]			ORIGINAL MEA	ORIGINAL MEASUREMENTS:				
			Coon, J.E.;	Auwaerter,	r, J.E.; McLaughlin, E 1989, 44, 305-345.			
			Fluid Phase	Equilibr.				
VARIABLES:			PREPARED BY:					
Temperature		W.E. Acree,	Jr.					
EXPERIMENTAL	VALUES							
T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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						

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:

COMPONENTS:			ORIGINAL MEASUREMENTS:											
(1) Xanthene; C ₁₃ H ₁₀ O; [92-83-1] (2) Benzene; C ₆ H ₆ ; [71-43-2] VARIABLES:			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E. J. Solution Chem. 1988, 16, 519-534. PREPARED BY:											
								Temperature			W.E. Acree, Jr.			
								EXPERIMENTAL V	VALUES		1			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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	Ī										
METHOD: APPARI	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:									
thermometer.	Constant temperature bath and a precision thermometer.			(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.										
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual														
noting the te	emperature at	which the last	ESTIMATED	ERRORS:										
crace or Boll	trace of solid solute disappeared.			T/K : precision \pm 0.1. x_1 : \pm 0.0003.										

COMPONENTS:		ORIGINAL MEASUREMENTS:				
 (1) Xanthene; C₁₃H₁₀O; [92-83-1] (2) 1,2,3,4-Tetrahydronaphthalene; C₁₀H₁₂; [119-64-2] 			Coon, J.E.; Auwaerter, J.E.; McLaughl: Fluid Phase Equilibr. 1989, 44, 305-			
Temperature		W.E. Acree	, Jr.			
EXPERIMENTAL 1	ALUES		-			
T/K	x ₂	<i>x</i> ₁	T/K	x ₂	<i>x</i> 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				
		AUXIL	ARY INFORMATION		• • • • • • • • • • • • • • • • • • • •	

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer. $% \left(1\right) =\left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left($

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:

COMPONENTS:			ORIGINAL M	Easurements:			
(1) Xanthene; C ₁₃ H ₁₀ O; [92-83-1] (2) Pyridine; C ₅ H ₅ N; [110-86-1]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E. J. Solution Chem. 1988, 16, 519-534. PREPARED BY: W.E. Acree, Jr.					
VARIABLES:							
Temperature							
EXPERIMENTAL '	VALUES						
T/K	x ₂	<i>x</i> ₁	T/K	<i>x</i> 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	1			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual			(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.				
noting the to		which the last	ESTIMATED	ERRORS:			
		•	T/K : precision \pm 0.1. x_1 : \pm 0.0003.				

COMPONENTS:		ORIGINAL MEASUREMENTS:											
(1) Xanthene; C ₁₃ H ₁₀ O; [92-83-1] (2) Thiophene; C ₄ H ₄ S; [110-02-1] VARIABLES: Temperature			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. 1988, 16, 519-534. PREPARED BY: W.E. Acree, Jr.										
								EXPERIMENTAL 1	VALUES		j		_
								T/K	<i>x</i> ₂	<i>x</i> ₁	T/K	<i>x</i> ₂	<i>x</i> 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: APPARA	ATUS/PROCEDUR	E	SOURCE AND P	URITY OF M	ATERIALS:								
thermometer.	Constant temperature bath and a precision thermometer.			(1) 99.65 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.									
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.										
			T/K: precis x ₁ : ± 0.000	ion <u>+</u> 0.1.									

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.

Fluoranthene

+	acenaphthene	13	
+	anthracene	11	
+	benzene	3, 4	
+	chlorobenzene	16	
+	2-chloro-1,3,5-trinitrobenzene	30	
+	chrysene	14	
+	cyclohexane	3	
+	2,7-dimethylnaphthalene	9	
+	dimethyl sulfoxide	20	
+	1,3-dinitrobenzene	21	
+	1,4-dinitrobenzene	22	
+	2,4-dinitromethylbenzene	25	
+	2,4-dinitrophenol	26	
+	1,4~dioxane	15	
+	ethanol	17	
+	fluorene	10	
+	1-hydroxy-2-methylbenzene	18	
+	methanol	16	
+	methylbenzene	5	
+	2-methylnaphthalene	8	
+	3-methyl-2,4,6-trinitrophenol	31	
+	naphthalene	7	
+	nitrobenzene	20	
+	1-octanol	17,	18
+	phenanthrene	12	
+	2-propanone	19	
+	pyridine	19	
+	tetrachloromethane	15	
+	1,2,4,5-tetramethylbenzene	6	
+	1,2,3,5-tetranitrobenzene	24	
+	2,4,6-trinitroaniline	29	
+	1,3,5-trinitrobenzene	23	
+	2,4,6-trinitromethoxybenzene	28	
+	2,4,6-trinitromethylbenzene	27	

Fluorene

+	acenaphthene	48
+	aniline	54
+	benzene	35-38
+	chlorobenzene	50
+	chrysene	49
+	cyclohexane	34
+	decahydronaphthalene	35
+	1,3-dimethylbenzene	41
+	1,4-dimethylbenzene	42
+	2,7-dimethylnaphthalene	46
+	1,2-dinitrobenzene	55
+	1,3-dinitrobenzene	56
+	1,4-dinitrobenzene	57
+	2,4-dinitromethylbenzene	60
+	2,4-dinitrophenol	62
+	ethanol	51
+	ethylbenzene	40
+	fluoranthene	47
+	methanol	51
+	methylbenzene	39

Fluorene		
	+ 2-methylnaphthalene	45
	+ 6-methyl-2,3,4-trinitrophenol	64
	+ naphthalene	44
	+ nitrobenzene	52
	+ 1-octanol	52
	+ pyridine	53
	+ tetrachloromethane	50
	+ 1,2,3,4-tetrahydronaphthalene	39
	+ 1,2,4,5-tetramethylbenzene	43
	+ 1,2,3,5-tetramethylbenzene + 1,2,3,5-tetranitrobenzene	59
	* * *	54
	+ thiophene	= -
	+ 1,3,5-trinitrobenzene	58
	+ 2,4,6-trinitromethylbenzene	61
	+ 2,4,6-trinitrophenol	63
Indole		
	+ benzene	66
	+ biphenyl	67, 68
	+ 2,6-dimethylnaphthalene	72
	+ diphenyl ether	73
	+ ethanol	74
	+ 2-methylindole	75
	+ 5-methylindole	76
	+ 1-methylnaphthalene	69
	+ 2-methylnaphthalene	70, 71
	+ quinoline	70, 71
	· darmorrue	/4
Naphthacene		
	+ benzene	78
	+ heptane	78
	+ 1-octanol	79
Naphthalene		
	+ acenaphthene	122
	+ acetonitrile	197
	+ aniline	171
	+ benzene	97-103, 193-196
	+ 1,2-benzenediol	164
	+ 1,3-benzenediol	165
	+ 1,4-benzenediol	163
	+ biphenyl	115
	+ 1-butanol	154-157
	+ 2-butanol	158
	+ 2-butanone	200
	+ butyl 2-furoate	125
	+ carbon disulfide	168
	+ chlorobenzene	140
	+ 1-chloro-3-nitrobenzene	175
	+ 1-chloro-4-nitrobenzene	176
	+ chrysene	121
	+ cyclohexane	89-93
	+ cyclohexanol	162
	+ decahydronaphthalene	97
	+ 1,1-dibromoethane	136
	+ 1,2-dibromoethane	137
	+ 1,4-dichlorobenzene	
	•	141
	+ 1,1-dichloroethane	138
	+ 1,2-dichloroethane	139
	+ dichloromethane	129
	+ diiodomethane	136
	+ 1,2-dimethylbenzene	112
	+ 1,3-dimethylbenzene	113, 195
	+ 1,4-dimethylbenzene	114
	+ cis-1,2-dimethylcyclohexane	94
		95
	+ trans-1,2-dimethylcyclohexane	95 96
		95 96 96

Naphthalene

+	trans-1,4-dimethylcyclohexane	95
+	2,2-dimethyloxetane	128
+	3,3-dimethyloxetane	128
+	2,4-dinitroaniline	177
+	1,3-dinitrobenzene	182, 183
+	3,5-dinitrobenzoic acid	178
+	2,4-dinitro-1-methylbenzene	187, 188
+	2,4-dinitrophenol	189
+	1,2-diphenylethane	116
+	1,2-ethanediol	201 147-150
+	ethanol	127
+	1-ethoxypropane	127
+	2-ethoxypropane ethylbenzene	108-111
+	ethyl ethanoate	202
+	ethyl 2-furoate	124
+	fluoranthene	119
+	fluorene	120
+	furfuryl acetate	123
+	furfuryl alcohol	166
+	heptane	87
+	hexadecane	88
+	hexafluorobenzene	142
+	hexane	83-86
+	1-hexanol	160, 199
+	indene	118
+	isoquinoline	191, 196
+	methanol	143-147, 198
+	methylbenzene	104-108, 193, 194
+	methylcyclohexane	94
+	methylcyclohexanol	163
+	methyl 2-furoate	124
+	2-methyl-1-propanol	158
+	2-methy1-2-propanol	159
+	2-nitrobenzaldehyde	172
+	3-nitrobenzaldehyde	173
+	4-nitrobenzaldehyde	174
+	nitrobenzene	169, 170
+	4-nitro-1-methylbenzene	180, 181 185
+	2-nitrophenol	186
+	4-nitrophenol	89
+	octadecane octafluoronaphthalene	142
+	octane	88
+	1-octanol	161, 162
+	1,1-oxybisbutane	126
	1,1-oxybisethane	126
+	1-pentanol	159
+	perfluoro-dibutyl ether	192
+	perfluoro-tripropylamine	192
+	1-propanol	150-152, 199
+	2-propanol	153
+	2-propanone	167, 200
+	propyl 2-furoate	125
+	4-isopropyl methylbenzene	117
+	pyrene	122
+	pyridine	172, 202
+	tetrachloromethane	131-135
+	1,2,3,4-tetrahydronaphthalene	117
+	tetrahydropyran	129
+	thiophene	171
+	trichloroethylene	135
+	trichloromethane	130, 131
+	1,3,5-trimethyl-2,4,6-	150
	trinitrobenzene	179

Naphthalene	+ 1,3,5-trinitrobenzene	184
	+ 2,4,6-trinitrophenol	190
	+ water	197-202
Perylene	+ benzene	204
	+ heptane	204
	+ 1-octanol	205
Phenanthrene		
Phenanthrene	+ acenaphthene	218
	+ benzene	213, 214
	+ benzoic acid	237
	+ biphenyl	216
	+ carbon disulfide	224
	+ 1-chloro-4-nitrobenzene	235
	+ trans-cinnamic acid	237
	+ cyclohexane	210-212
	 decahydronaphthalene 	213
	+ dibenzothiophene	235
	+ 1,8-dihydroperfluorooctane	220
	+ 1,4-dibromobenzene	219
	+ 1,2-dinitrobenzene	225
	+ 1,3-dinitrobenzene	226
	+ 1,4-dinitrobenzene	227
	+ 2,4-dinitromethylbenzene	230
	+ 2,6-dinitromethylbenzene	231
	+ 3,4-dinitromethylbenzene	232
	+ 2,4-dinitrophenol	234
	+ ethanol	221
	+ fluoranthene	217
	+ heptane	208, 209
	+ hexane	208
	+ 1-hydroperfluoroheptane	220
	+ 2-hydroxybenzoic acid	238
	 3-hydroxybenzoic acid 	239
	+ methylbenzene	214, 215
	+ 6-methyl-2,3,4-trinitrophen	
	+ nitrobenzene	224
	+ octane	209
	+ octadecane	210
	 octafluoronaphthalene 	221
	+ 1-octanol	222
	+ perfluoro-tri-n-butylamine	223
	+ pyridine	222
	+ tetrachloromethane	219
	+ 1,2,3,4-tetrahydronaphthale	
	+ 1,2,3,5-tetranitrobenzene	229
	+ thianthrene	236
	+ thiophene	223
	+ 1,3,5-trinitrobenzene	228
	+ 2,4,6-trinitromethylbenzene	233
1,10-Phenanthro	line	
	+ ethanol	244
	+ methanol	242, 243
	+ water	242-244
Phenothiazine		
ruenochiazine	+ dibenzo[b,e][1,4]dioxine	249
	+ phenoxanthiin	248
	+ phenoxarine	246
	· Pucuovarrue	247

Phenoxanthiin		
	+ dibenzo[b,e][1,4]dioxin	253
	+ phenothiazine	252
	+ phenoxazine	251 251
	+ thianthrene	231
Phenoxazine		
	<pre>+ dibenzo[b,e][1,4]dioxin</pre>	257
	+ phenothiazine	255
	+ phenoxanthiin	256 256
	+ thianthrene	250
Pyrene		
	+ acetonitrile	287
	+ benzene	266 280
	+ 1-butanol	281
	+ 2-butanol	265
	<pre>+ t-butylcyclohexane + butyl ethanoate</pre>	272
	+ butyl ethanoate + 1-chlorobutane	276
	+ 2-chloro-1,3,5-trinitrobenzene	297, 298
	+ chrysene	270
	+ cyclohexane	262, 263, 303, 30
	+ cyclooctane	264
	+ cyclopentanol	284
	+ 1,4-dichlorobutane	276
	+ 1,2-dichloroethane	275
	+ 1,2-dimethylbenzene	268
	+ 1,3-dimethylbenzene	269
	+ 1,4-dimethylbenzene	269
	+ dimethyl sulfoxide	286
	+ 1,3-dinitrobenzene	288 .
	+ 1,4-dinitrobenzene	289 292
	+ 2,4-dinitromethylbenzene	292
	+ 2,4-dinitrophenol + 1,4-dioxane	273, 274
	+ ethanol	278, 279
	+ ethanol + ethyl butyrate	272
	+ ethyl ethanoate	271
	+ heptane	260, 261, 301, 30
	+ hexane	260, 300, 306
	+ 1-hydroxy-2-methylbenzene	284
	+ methanol	277, 278
	+ methylbenzene	267, 268
	+ 3-methyl-1-butanol	282
	+ methylcyclohexane	264, 304, 310
	+ 2-methyl-1-propanol	282
	+ 3-methyl-2,4,6-trinitrophenol	299
	+ naphthalene	271
	+ octadecane	262 277
	+ octafluoronaphthalene	261, 302, 308
	+ octane + 1-octanol	283
		273
	+ 1,1-oxybisbutane + 1-pentanol	281
	+ 1-propanol	279, 300-305
	+ 2-propanol	280, 306-311
	+ 2-propanone	285
	+ pyridine	286
	+ tetrachloromethane	274, 275
	+ 1,2,3,5-tetranitrobenzene	291
	+ 2,2,4-trimethylpentane	265, 305, 311
	+ 2,4,6-trinitroaniline	296
	+ 1,3,5-trinitrobenzene	290
	+ 2,4,6-trinitromethoxybenzene	295
	+ 2,4,6-trinitromethylbenzene	294

Thianthene	+ cyclohexane	314
	<u>=</u>	315
	,	313
	+ heptane	313
	+ hexane	315
	+ methylcyclohexane	314
	+ octane	314
	+ phenanthrene	317
	+ phenothiazine	318 319
	+ phenoxanthiin	319 319
	+ phenoxazine	
	+ 2,2,4-trimethylpentane	316
Thioxanthene		
	+ benzene	322
	+ cyclohexane	321
	 decahydronaphthalene 	321
	+ pyridine	323
	+ 1,2,3,4-tetrahydronaphthalene	322
	+ thiophene	323
Triphenylene		
	+ benz[a]anthracene	326
	+ benzene	325
	+ , heptane	325
Xanthene		
	+ benzene	329
	+ cyclohexane	328
	+ decahydronaphthalene	328
	+ pyridine	330
	+ 1,2,3,4-tetrahydronaphthalene	329
	+ thiophene	330

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.

51-28-5	26, 62, 189, 234, 293
56-23-5	15, 50, 131-135, 219, 274, 275
56-55-3	326
60-29-7	126
62-53-3	54, 171
64-17-5	17, 51, 74, 147-150, 221, 244, 278, 279
65-85-0	237
67-56-1	16, 51, 143-147, 197, 242, 243, 277,
	278
67-63-0	153, 280, 306-311
67-64-1	19, 167, 200, 285
67-66-3	130, 131
67-68-5	20, 286
69-72-7	238
71-23-8	150-152, 199, 279, 300-305
71-36-3	154-157, 280
71-41-0	159, 281
71-43-2	3, 4, 35-38, 66, 78, 97-103, 193-196,
	204, 213, 214, 266, 322, 325, 329
75-05-8	197, 287
75-09-2	129
75-11-6	136
75-15-0	168, 224
75-34-3	138
75-65-0	159
78-83-1	158, 282
78-93-3	200
79-01-6	135
83-32-9	13, 48, 122, 218
85-01-8	12, 208-240, 317
86-73-7	10, 34-64, 120
88-75-5	185
88-88-0	30, 297, 298
88-89-1	63, 190
90-12-0	69

91-17-8	35, 97, 213, 321, 328
91-20-3	7, 44, 83-202, 271
91-22-5	74
91-57-6	8, 45, 70, 71
92-24-0	78, 79
92-52-4	67, 68, 115, 216
92-83-1	328-330
92-84-2	246-249, 252, 255, 318
92-85-3	236, 247, 251, 256, 313-319
95-13-6	118
95-20-5	75
95-47-6	112, 268
95-48-7	18, 284
95-93-2	6, 43
96-41-3	284
97-02-9	177
98-00-0	166
98-95-3	20, 52, 169, 170, 224
99-06-9	239
99-34-3	178
99-35-4	23, 58, 184, 228, 290
99-61-6	173
99-65-0	21, 56, 182,183, 226, 288
99-87-6	117
99-99-0	180, 181
100-00-5	176, 235
100-02-7	186
100-25-4	22, 57, 227, 289
100-41-4	40, 108-111
101-84-8	73
103-29-7	116
105-54-4	272
106-37-6	219
106-42-3	42, 114, 269
106-46-7	141
106-93-4	137
107-06-2	139, 275
107-21-1	201
108-38-3	41, 113, 195, 269
108-46-3	165
108-87-2	94, 264, 304, 310, 315

108-88-3	5, 39, 104-108, 193, 194, 214, 215,
	267, 268
108-90-7	16, 50, 140
108-93-0	162
109-69-3	276
110-02-1	54, 171, 223, 323, 330
110-54-3	83-86, 208, 260, 300, 306, 313
110-56-5	276
110-82-7	3, 34, 89-93, 210-212, 262, 263, 303,
	309, 314, 321, 328
110-86-1	19, 53, 172, 222, 286, 323, 330
111-27-3	160, 199
111-65-9	88, 209, 261, 302, 308, 314
111-87-5	17, 18, 52, 79, 161, 162, 205, 222, 283
118-96-7	27, 61, 233, 294
119-64-2	39, 117, 216, 322, 329
119-65-3	191, 196
120-12-7	11
120-72-9	66-76
120-80-9	164
121-14-2	25, 60, 187, 188, 230, 292
121-73-3	175
123-31-9	163
123-51-3	282
123-86-4	272
123-91-1	15, 273, 274
129-00-0	122, 260-311
132-65-0	235
135-67-1	246, 251, 255-257, 319
140-10-3	237
141-78-6	202, 271
142-68-7	129
142-82-5	78, 87, 204, 208, 209, 260, 261, 301,
	307, 313, 325
142-96-1	126, 273
198-55-0	204, 205
206-44-0	3-31, 47, 119, 217
217-59-4	325, 326
218-01-9	14, 49, 121, 270
261-31-4	321-323
262-12-4	249, 253, 257
262-20-4	248, 251-253, 256, 319

١		
	292-64-8	264, 315
	307-99-3	220
١	308-48-5	192
	311-89-7	223
	313-72-4	142, 221, 277
	338-83-0	192
	375-83-7	220
I	392-56-3	142
	489-98-5	29, 296
Ì	528-29-0	55, 225
	540-84-1	265, 305, 311, 316
	544-76-3	88
	552-89-6	172
	555-16-8	179
	557-91-5	136
Ì	581-42-0	72
١	582-16-1	9, 46
I	583-33-5	125
١	593-45-3	89, 210, 262
l	602-96-0	174
İ	602-99-3	31, 299
١	606-20-2	231
	606-35-9	28, 295
١	610-39-9	232
	611-13-2	124
ı	614-96-0	76
	614-99-3	124
l	615-10-1	125
l	623-17-6	123
	624-29-3	96
	625-54-7	127
l	628-32-0	127
l	638-04-0	96
l	2207-01-4	94
	2207-04-7	95
l	3178-22-1	265
l	3698-53-1	24, 59, 229, 291
	5144-89-8	242-244
	6245-99-4	128
١	6876-23-9	95
	6921-35-3	128
	7732-18-5	197-202, 242-244

 15892-23-6
 158, 281

 25639-42-3
 163

 89793-90-8
 64, 240

.

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.

78, 87, 204, 208, 261, 325 Abuin, E.B. xvi, xviii, xxvi, 36, 83, 86, 89, Acree, W.E., Jr. 90, 97-99, 104, 108-110, 132, 135, 143, 148, 151, 154, 211, 260-262, 264-266, 268, 269, 271-276, 278-285, 300-311, 313-316 xxv Adjei, A. 243 Amalendu, P. 146, 150, 152, 157, 159 Andren, A.W. 146, 150, 152, 157, 159 Armstrong, D.E. 122, 142, 221, 271, 277 Asakawa, T. 35, 39, 97, 117, 213, 216, 321-323, Auwaerter, J.E. 328-330 298 Bando, M. Barton, A.F.M. xxiii 244 Battacharyya Beerbower, A. xxv Belloto, R.J., Jr. xxvi 126-129 Bennett, G.M. Braton, C.M. 263, 267, 272, 287 Brennecke, J.F. 235 Bryant, H.W. 34, 35, 92, 100, 210, 213 Buehring, K.G. 235 Burger, A. 242 Burgess, J. Carre, O.R. 263, 267, 272, 287 xxiv, 84, 87, 88, 93-96, 101, 105, Chang, W. 110, 129, 130, 133, 137-140, 168 Chickos, J.S. xxi Chiou, C.T. xxii 34, 35, 53, 54, 92, 100, 171, 172, Choi, P.B. 210, 213, 215, 222, 223 Cline, P.V. 15, 16, 18, 20, 135, 146, 273, 277, 284, 286 Connors, K.A. 197, 198, 201 Cook, W.A. 141 Coon, J.E. 35, 39, 97, 117, 213, 216, 321-323, 328-330 Cullinane, N.M. 246-249, 251-253, 255-257, 318, 319 74 Dehn, W.M. 190 Dhillon, M.S. Dickhut, R.M. 146, 150, 152, 157, 159 Djordjevic, N.M. 89, 210, 262 Doane, E.P. 208, 209, 224 38, 85, 92, 136, 149, 155, 160, 161 Domanska, U. Drickamer, H.G. 208, 209, 224 Ebina, T. 66, 67, 69, 70, 75, 76 236, 238, 239, 317 Eckert, C.A.

```
64, 240
Efremov, N.N.
                                            64, 240
Fikhomirova, A.N.
Gomes de Azevedo, E.
                                            xvii
Gordon, L.G.
                                            212
Grant, D.J.W.
                                            xvi
Groves, F.R., Jr.
                                            38
Gupta, P.D.
                                            169, 224
Haines, R.I.
                                            242
Hammick, D.L.
                                            179
Hellicar, A.
                                            179
                                           84, 88, 90, 91, 100, 105, 108, 131,
Heric, E.L.
                                            133
Hesse, D.G.
                                            xxi
                                            xvi
Higuchi, T.
Hildebrand, J.H.
                                           xvii
Hofmeier, F.
                                           234
Howell, W.J.
                                           236, 238, 239, 317
Hoy, K.L.
                                           xxiii
Huang, G.-L.
                                           17-30, 52, 79, 162, 205, 222, 283
Isomi, A.
                                           122, 142, 221, 271, 277
                                           122, 142, 221, 271, 277
Iwata, T.
James, K.C.
                                            xvii
                                            163-165
Janetzky, E.
Judy, C.L.
                                           86, 89, 97, 108, 110, 135, 260-262;
                                           264-266
Khossravi, D.
                                            197, 198, 201
                                            180, 187
Kofler, A.
                                           298
Krajewska, A.
Kravchenko, V.M.
                                            4, 6-14, 40, 41, 43-49, 103, 107,
                                           111-114, 118-122, 191, 193-196, 217,
                                           218, 270
                                           55-58, 60-63, 163-165, 170, 181,
Kremann, R.
                                           183-186, 188, 189, 225-228, 230-234
                                           5, 17, 19, 267, 278, 285, 286
Krezewki, R.
Lahiri, S.C.
                                           243, 244
Lawe, T.
                                           15, 16, 18, 20, 115, 116, 135, 146,
Lee, L.S.
                                           273, 277, 284, 286
                                           xvii
Lichtenthaler, R.N.
                                           xxi
Liebman, J.F.
Linevsky, M.J.
Lissi, E.A.
                                           78, 87, 204, 208, 261, 325
                                           17-30, 52, 79, 162, 205, 222, 283<sup>-</sup>
Mackay, D.
Mahieu, J.
                                           126, 130, 168
                                           xxii
Manes, M.
Martin, A.
                                           xxv
Matsunaga, Y.
                                           298
Mayer, M.M.
                                           236, 238, 239, 317
McCargar, J.W.
                                           xxvi
McLaughlin, E.
                                           3, 15, 34, 35, 37-39, 50, 53, 54,
                                           92, 93, 97, 100, 101, 117, 134, 142,
                                           171, 172, 210, 212-216, 219,220,
                                           222, 223, 263, 266, 274, 321-323,
                                           325, 328-330
Messer, C.E.
                                           142
Miller, M.M.
                                           17-30, 52, 79, 162, 205, 222, 283
```

79, 204 Mishra, D.S. 122, 142, 221, 271, 277 Miyaqishi, S. Morris, R.E. 141 Mortimer, F.S. 37, 39, 42, 50-54 264, 265, 273 Murral, D.J. Newberger, J. xxv Nigam, R.K. 190 Nishida, M. 122, 142, 221, 271, 277 Ochsner, A.B. xxvi Okamoto, K. 182 Oswalt, B.M. 264, 265, 273 Pastukhova, I.S. 4, 6-14, 47-49, 103, 107, 111-114, 118, 119, 121, 122, 191, 196, 217, 218, 270 xix Pemenzi, O. Philip, W.G. 126-129 Phillips, D.J. 263, 267, 272, 287 Pinal, R. 15, 16, 18, 20, 135, 146, 273, 277, 284, 286 Pontikos, N.M. 86, 89, 97, 108, 110, 135, 260-262, 264-266 Posey, C.D. 84, 88, 91, 100, 105, 108, 131 Powell, J.R. 268, 269, 271, 272, 274-276, 278-285 Prausnitz, J.M. xvii, xviii, xxv Pucher, G. 74 Rai, U.S. 216, 219, 235, 237 Rao, P.S.C. 15, 16, 18, 20, 135, 146, 273, 277, 284, 286 Rees, W.T. 246-249, 251-253, 255-257, 318, 319 Rosenblum, C. 136-139 Sabbah, R. xix Salazar, A. 268, 269, 271, 272, 274-276, 278-285 Sarker, M. 199, 200, 202 Scott, R.L. xvii, 212, 220, 223 Sediawan, W.B. 321-323, 328-330 Sekiguchi, K. 182 Sengupta, D. 243, 244 Shekhar, H. 216, 219, 235, 237 Shinoda, K. xvii Shinomiya, C. 21-31, 59, 172-178, 229, 288-297, Shirotani, K .- I. 182 Shiu, W.-Y. 17-30, 52, 79, 162, 205, 222, 283 Simons, J.H. 192 Smutek, M. 5, 17, 19, 267, 278, 285, 286 Sokoloski, T.D. xxvi Speyers, C.L. 106, 131, 147, 152, 214, 221 Srivastava, R.D. 169, 224 Sturrock, M.G. 326 Sunier, A.A. 123-125, 136-139, 145, 149, 150, 153, 157-159, 166 Suzuki, E. 182 Szafranski, A.M. 68, 71-73 Takahashi, S. 66, 67, 69, 70, 75, 76 Teng, I.-L. xxvi Tomasko, D.L. 236, 238, 239, 317

Tsuda, Y.
Tucker, S.A.
Valvani, S.C.
Voisinet, D.
Wallach, J.R.
Ward, H.L.

Warner, J.C.
Wasik, S.P.
Wasilewska, K.
Weimer, R.F.
Weissenberger, G.
Wheeler, A.S.
Williams, C.P.
Wilson, D.
Wu, P.L.

Wyrzykowska-Stankiewicz, A.M. Yalkowsky, S.H.

Yeh, K.-N. Yokoyama, C. Zainal, H.A.

Zvaigzne, A.I.

182 264, 265, 273, 276, 313-316 268, 269, 271, 272, 274-276, 278-285 264, 265, 273 83, 86, 102, 106, 115, 116, 134, 140, 144, 156, 167, 169, 171 115, 116 17-30, 52, 79, 162, 205, 222, 283 298 xviii 162, 163 117 34, 35, 92, 100, 210, 213 199, 200, 202 xxv 68, 71-73 xx, 15, 16, 18, 20, 78, 135, 146, 204, 273, 277, 284, 286 91, 133 66, 67, 69, 70, 75, 76 3, 15, 34, 37, 50, 93, 101, 134, 212, 214, 219, 263, 266, 274, 325

xxvi, 276, 279, 280, 300-311, 313-

316

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Volume 1	H. L. Clever, Helium and Neon
Volume 2	H. L. Clever, Krypton, Xenon and Radon
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	Part II: Esters 7-C to 32-C
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	Than 200 kPa
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	Solvents
Volume 55	S. Siekierski and S. L. Phillips, Actinide Nitrates
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	Hydrocarbons
Volume 57	W. Hayduk, Ethene
Volume 58	W. E. Acree, Jr, Polycyclic Aromatic Hydrocarbons: Binary Non-aqueous
	Systems. Part I: Solutes A–E