# INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

# ANALYTICAL CHEMISTRY DIVISION COMMISSION ON SOLUBILITY DATA

# **SOLUBILITY DATA SERIES**

Volume 58

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

# SOLUBILITY DATA SERIES

Editor-in-Chief
J.W. Lorimer
The University of Western Ontario
London, Ontario, Canada

M.-T. Saugier-Cohen Adad Sub-editor Solid/Liquid Systems C.L. Young
Sub-editor
Indexes

# **EDITORIAL BOARD**

H. Gamsjäger (Austria)
H.L. Clever (USA)
F.W. Getzen (USA)
A.F. Danil de Namor (UK)
J. Eysseltová (Czech Republic)
J.B. Jensen (Denmark)

C. Kalidas (India)
M. Salomon (USA)
D.G. Shaw (USA)
H. Miyamoto (Japan)
R.P.T. Tomkins (USA)
V.M. Valyashko (Russia)
J. Vanderdeelen (Belgium)

Managing Editor

P.D. Gujral

IUPAC Secretariat, Oxford, UK

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY IUPAC SECRETARIAT: Bank Court Chambers, 2-3 Pound Way Templars Square, Cowley, Oxford OX4 3YF, UK

# **SOLUBILITY DATA SERIES**

# Volume 58

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

Volume Editor

W. E. Acree, Jr.

University of North Texas Denton, Texas, USA

# **IUPAC Solubility Data Series Rates for 1995**

Subscriptions: UK and Europe Rest of World

Full subscription £265 \$395
Single volume £80 \$120

Reduced rates are available to members of IUPAC. Please apply directly to the publisher for details.

Prices include postage by surface mail or, for subscribers in the USA and Canada by Airfreight or in Japan, India, Australia and New Zealand by Air Speeded Post. Airmail rates are available on request.

The IUPAC Solubility Data Series is published quarterly in March, June, September and December by Oxford University Press. Subscription is \$395 per year. Second Class postage paid at Newark, New Jersey. ISSN 0191-5622.

POSTMASTER: Send address corrections to IUPAC Solubility Data Series, c/o Virgin Mailing and Distribution, Cargo Atlantic, 10 Camptown Road, Irvington, New Jersey 07111-1105, USA.

New subscriptions may be registered at any time during the year but will be reckoned as running from January 1st of the year in which the subscription is received. Claims regarding non-receipt of issues must be received within 4 months of publication or date of order, whichever is later. Back issues are available—for information contact Journals Customer Services Department, Oxford University Press, Walton Street, Oxford OX2 6DP.

#### **Order Information**

Payment is required with all orders and may be made by the following methods:

Cheque (made payable to Oxford University Press)

National Girobank (Account 500 1056)

Credit Card (Access, Visa, American Express, Diners Club)

Direct Debit: Please send for further details

**UNESCO Coupons** 

Bankers: Barclays Bank plc, PO Box 333, Oxford

Code 20-65-18. Account 00715654

Please send orders to: Journals Subscription Department, Oxford University Press, Walton

Street, Oxford OX2 6DP. Tel: +44(0)1865 56767, Fax: +44(0)1865 267773

Any enquires regarding this publication should be addressed to:

USA and Canada: Oxford University Press, 2001 Evans Road, Cary, NC 27513, USA. Rest of World: Journals Customer Services Department, Oxford University Press, Walton Street, Oxford OX2 6DP, UK.

O1995 International Union of Pure and Applied Chemistry. All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior written permission of the Copyright owner.

# CONTENTS

	Introduction to the Solubility of Solids in Liquids	viii
	Preface	жv
	Basic Thermodynamic Principles	xvii
	Scatchard-Hildebrand Solubility Parameter Model	xxiii
	Mobile Order Theory for Binary Alkane + Alcohol Solvent Mixtures	xxvi
	Mobile Order Theory for Binary Alcohol + Alcohol Solvent Mixtures	xxxiv
	Mathematical Representation of Solubility Data in Binary Solvents	xxxvi
	References	xliv
1	Acenaphthene Solubilities in Pure and Binary Solvent Mixtures	1
	Saturated Hydrocarbons (including Cycloalkanes)	2
	Aromatic Hydrocarbons	4
	Haloalkanes and Haloaromatic Hydrocarbons	17
	Alcohols	18
	Miscellaneous Pure Solvents	20
2	Acridine Solubilities in Pure and Binary Solvent Mixtures	22
	Saturated Hydrocarbons (including Cycloalkanes)	23
	Aromatic Hydrocarbons	24
	Miscellaneous Pure Solvents	25
3	Anthracene Solubilites in Pure and Binary Solvent Mixtures	26
	Saturated Hydrocarbons (including Cycloalkanes)	29
	Aromatic Hydrocarbons	37
	Esters	47
	Ethers	50
	Haloalkanes and Haloaromatic Hydrocarbons	54
	Alcohols	60
	Ketones	69
	Micellaneous Pure Solvents	71
	Binary Solvent Mixtures	84
4	Benz[a]anthracene Solubilities in Pure and Binary Solvent Mixtures	145
	Saturated Hydrocarbons (including Cycloalkanes)	146
5	Benzo[b]fluorene Solubilities in Pure and Binary Solvent Mixtures	147
	Alcohols	148
6	Benzo[ghi]perylene Solubilities in Pure and Binary Solvent Mixtures	149
	Saturated Hydrocarbons (including Cycloalkanes)	150
	Aromatic Hydrocarbons	151
	Esters	151
•	Ketones	152
7	Benzo[a]pyrene Solubilities in Pure and Binary Solvent Mixtures	154
	Saturated Hydrocarbons (including Cycloalkanes)	155
	Aromatic Hydrocarbons	155

8	Biphenyl Solubilities in Pure and Binary Solvent Mixtures	156
	Saturated Hydrocarbons (including Cycloalkanes)	158
	Aromatic Hydrocarbons	174
	Ethers	182
	Haloalkanes and Haloaromatic Hydrocarbons	184
	Alcohols	192
	Ketones	194
	Miscellaneous Pure Solvents	195
9	2,2'-Bipyridine Solubilities in Pure and Binary Solvent Mixtures	202
	Binary Solvent Mixtures	203
10	Buckminsterfullerene Solubilities in Pure and Binary Solvent Mixtures	206
	Saturated Hydrocarbons (including Cycloalkanes)	208
	Aromatic Hydrocarbons	212
	Ethers	224
	Haloalkanes and Haloaromatic Hydrocarbons	225
	Alcohols	237
	Miscellaneous Pure Solvents	237
11	Carbazole Solubilities in Pure and Binary Solvent Mixtures	243
	Saturated Hydrocarbons (including Cycloalkanes)	245
	Aromatic Hydrocarbons	256
	Esters	259
	Ethers	260
	Haloalkanes and Haloaromatic Hydrocarbons	265
	Alcohols	269
	Ketones	275
	Miscellaneous Pure Solvents	277
12	Chrysene Solubilities in Pure and Binary Solvent Mixtures	286
	Saturated Hydrocarbons (including Cycloalkanes)	287
	Aromatic Hydrocarbons	287
	Alcohols	296
	Miscellaneous Pure Solvents	297
13	Coronene Solubilities in Pure and Binary Solvent Mixtures	299
	Saturated Hydrocarbons (including Cycloalkanes)	300
	Alcohols	300
14	Dibenz[a,h]anthracene Solubilities in Pure and Binary Solvent Mixtures	301
	Saturated Hydrocarbons (including Cycloalkanes)	302
	Alcohols	302
15	Dibenzofuran Solubilities in Pure and Binary Solvent Mixtures	303
	Saturated Hydrocarbons (including Cycloalkanes)	304
	Aromatic Hydrocarbons	305
	Miscellaneous Pure Solvents	307
16	Dibenzothiophene Solubilities in Pure and Binary Solvent Mixtures	308
	Saturated Hydrocarbons (including Cycloalkanes)	309

	Aromatic Hydrocarbons	310
	Miscellaneous Pure Solvents	312
17	1,2-Diphenylbenzene Solubilities in Pure and Binary Solvent Mixtures	313
	Saturated Hydrocarbons (including Cycloalkanes)	314
	Aromatic Hydrocarbons	314
	Haloalkanes and Haloaromatic Hydrocarbons	315
18	1,3-Diphenylbenzene Solubilities in Pure and Binary Solvent Mixtures	316
	Saturated Hydrocarbons (including Cycloalkanes)	317
	Aromatic Hydrocarbons	317
	Haloalkanes and Haloaromatic Hydrocarbons	318
19	1,4-Diphenylbenzene Solubilities in Pure and Binary Solvent Mixtures	319
	Aromatic Hydrocarbons	320
Syst	cem Index	321
Reg.	istry Number Index	327
Aut	hor Index	332
Sol	ubility Data Series: Published and Forthcoming Volumes	337

### 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: The to the end of the known elements, in order of atomic number.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

#### **Evaluations**

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

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

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

Critical Evaluation:

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

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

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

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

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

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

# QUANTITIES AND UNITS USED IN COMPILATION AND EVALUATION OF SOLUBILITY DATA

#### Mixtures, Solutions and Solubilities

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

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

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

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

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

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

# Physicochemical Quantities and Units

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

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

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

$$x_1 = n_1 / \sum_{s=1}^{c} n_s$$
 [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  $\nu_{i+}$  cations and  $\nu_{i-}$  anions, with  $\nu_{i} = \nu_{i+} + \nu_{i-}$  and a mixture of p non-electrolytes k, of which some may be considered as solvent components, a generalization of the definition in (7) gives:

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

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

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

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

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

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

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

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

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

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

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

SI base units: mol kg<sup>-1</sup>. 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<sup>-1</sup>. 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,  $\rho_1$ :

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

SI base units: kg m<sup>-3</sup>.

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  $z_+$ ,  $z_-$ ,

$$I_m = |z_+ z_-| v m_i, \quad I_c = |z_+ z_-| v c_i$$
 [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.

#### REFERENCES

- 1. Hill, E.A. J. Am. Chem. Soc. 1900, 22, 478.
- IUPAC Commission on Atomic Weights and Isotopic Abundances. Pure Appl. Chem. 1989, 63, 975.
- Mills, I.; et al., eds. Quantities, Units and Symbols in Physical Chemistry (the Green Book). Blackwell Scientific Publications. Oxford, UK. 1993.
- 4. Ku, H.H., p. 73; Eisenhart, C., p. 69; in Ku, H.H., ed. Precision Measurement and Calibration. NBS Special Publication 300. Vol. 1. Washington. 1969.
- 5. Gold, V.; et al., eds. *Compendium of Analytical Nomenclature* (the *Gold Book*). Blackwell Scientific Publications. Oxford, UK. 1987.
- 6. Freiser, H.; Nancollas, G.H., eds. *Compendium of Analytical Nomenclature* (the *Orange Book*). Blackwell Scientific Publications. Oxford, UK. 1987. Sect. 9.1.8.
- 7. Robinson, R.A.; Stokes, R.H. Electrolyte Solutions. Butterworths. London. 1959. 2nd ed.
- 8. Jänecke, E. Z. Anorg. Chem. 1906, 51, 132.
- 9. Friedman, H.L. J. Chem. Phys. 1960, 32, 1351.
- Lorimer, J.W. in Cohen-Adad, R.; Lorimer, J.W. Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems). IUPAC Solubility Data Series, Vol. 47. Pergamon Press. Oxford, UK, 1991. p. 495.

R. Cohen-Adad Villeurbanne, France

J.W. Lorimer London, Ont., Canada

M. Salomon Sea Bright, NJ, USA

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

January, 1994

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

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

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

#### PREFACE

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

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

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

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

Polycyclic aromatic compounds are an important chemical class. They have been used as model compounds in coal liquefaction process design calculations, serve as the "parent" compound or base found in a number of drug molecules, and several are mutagens, carcinogens, or common organic pollutants resulting from oil spills.

Moreover, many of the polycyclic aromatic compounds have very limited mole fraction solubilities, and from a thermodynamic modeling standpoint, saturated solutions are treated as infinitely dilute solutions. The solute is considered to be surrounded by solvent molecules. Solute-solute molecular interactions are ignored.

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

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

Hildebrand and Scott (3), James (4), Prausnitz et al. (5), and Shinoda (6).

#### BASIC THERMODYNAMIC PRINCIPLES

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

$$c_i = [i] = n_i/V$$
 SI base units: mol dm<sup>-3</sup> [1]

(3) mole 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  $V_{m,1}$  (molar mass divided by density)

$$\phi_1 = n_1 V_{m,1}/(n_1 V_{m,1} + n_2 V_{m,2} + n_3 V_{m,3} + \dots)$$
 [4] as this quantity serves as an input parameter in expressions for estimating solubilities in mixed solvents since it requires no a priori knowledge concerning volumetric behavior. Solute solubilities can be found in the chemical literature in terms of any of the aforementioned concentration variables, or as molality,  $m_i$ , which is the amount of solute  $\underline{i}$  divided by the mass of the solvent

$$m_{\rm i} = n_{\rm i}/n_{\rm s} \, \rm M_{\rm s}$$
 SI base unit: mol kg<sup>-1</sup> [5] where M<sub>e</sub> is the molar mass of the solvent.

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

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

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

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

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

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

$$\mathbf{a}_1 = \mathbf{a}_1^* \tag{6}$$

or

$$a_1^* = \gamma_1 x_1 a_1^0$$
 [7]

where \* is the pure solid,  $x_1$  is the mole fraction solubility of the solute in the solvent,  $\gamma_1$  is the liquid-phase activity coefficient and  $a_1^{\circ}$  is the standard state activity to which  $\gamma_1$  refers. Selection of the standard state  $a_1^{\circ}$  is arbitrary, the only thermodynamic requirement being that it must be at the same temperature as the saturated solution. For thermodynamic modeling of nonelectrolyte solutions, it is advantageous to define the standard state activity as the activity of the pure supercooled liquid,  $a_1^{*}(1)$ , at the solution's temperature and some specified pressure. Although this is a hypothetical standard state, it is one whose properties can be calculated with reasonable accuracy provided that the solution's temperature is not too far removed from the melting point temperature of the solute,  $T_{MD}$ .

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

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

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

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

with the overall process being

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

and

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

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

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

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

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

TABLE I. Enthalpies and Entropies of Fusion of Select Polycyclic Aromatic Hydrocarbons and Hetero-atom Derivatives<sup>a</sup>

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

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

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

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

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

As noted by the authors, the molar entropy of fusion,  $\Delta S^{\text{fus}}$ , is equal to the entropy of the liquid state minus the entropy of the crystal

$$\Delta S^{\text{fus}} = -R \ln P^{\text{fus}} \tag{10}$$

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

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

The translational entropy was visualized by a two-dimensional analogy involving a field of checkers or disks that had been trapped into a nearly closest-packed two-dimensional crystalline arrangement. When the crystal melts, a slight expansion and randomization of the disk positions occur. The probability of two-dimensional fusion is equal to the total number of arrangements of the disks that are possible within the area allotted for the solid divided by the corresponding number of arrangements that are possible within the area allotted to the liquid melt. This, in turn, is related to the ratio of the free areas available within each phase for the disks to occupy. Free areas are replaced by free volumes in the case of a three-dimensional arrangement of molecules. Entropies of fusion for spherical molecules such as inert gases and for pseudospherical molecules such as tetrachloromethane typically range between 12.5 - 16.7 J mol<sup>-1</sup> K<sup>-1</sup>. Yalkowsky and Valvani (11) assumed the intermediate value of AS<sup>trans</sup> = 14.6 J mol<sup>-1</sup> K<sup>-1</sup> 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 webble or vibrate approximately  $10^{\circ}$  in the spherical coordinates  $\phi$  and  $\theta$  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  $\phi$  and  $\theta$ . 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  $\phi$  and  $\theta$  corresponds to a spherical segment that is roughly 0.00754 times that of a sphere of the same radius, or roughly a rotational entropy of fusion of  $\Delta S^{fus} = 41.8 \text{ J mol}^{-1}$  K<sup>-1</sup>. On the basis of the above discussion, the total entropy of fusion for a rigid polycyclic aromatic compound would be  $\Delta S^{fus} = \Delta S^{trans} + \Delta S^{rot} \approx 56.4 \text{ J mol}^{-1}$  K<sup>-1</sup>, which is in reasonable (though by no means perfect) agreement with experimental values listed in Table I.

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

For acyclic and aromatic hydrocarbons

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

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

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

where  $K = \sum_{i=1}^{n} n_{k}$ , n refers to the number of equivalent methylene groups necessary to simulate the size of the ring, R is the total number of ring atoms and N indicates the total number of rings in the polycyclic molecule. Hydrocarbon components are identified by the subscript i, the j subscript identifies the carbon(s) bearing the functional group(s) and the k subscript denotes the different functional groups in the molecule. Each group contribution to the entropy of fusion represents the product of the number of identical groups in the molecule (n) times the group value (G) times an empirical coefficient (C) which modifies each group contribution according to the structural environment around the carbon atom bearing substituent functional groups.

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

approximately 7 %.

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

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

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

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

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

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

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

Chiou and Manes (15) compared experimental solubilities of 11 crystalline nonpolar polycyclic aromatic compounds and their derivatives in glycerol trioleate ( $V_{m,s}$  = 966 cm<sup>3</sup> mol<sup>-1</sup>) to predictions based upon eqns. [9] and [17]. The authors' calculations revealed that the observed mole fraction solubilities are considerably higher than the predictions of eqn. [9] (with  $\Delta C_p$  = 0); the predictions in some instances being low by as much as 100 percent. In comparison, the observed volume fraction solubilities,  $\phi_1$ , were comparable to or only slightly lower than the predictions of eqn. [17] (again with  $\Delta C_p$  = 0). The magnitude of the deviations from Raoult's law is well beyond the uncertainty of the observed solubilities. Since the solubility data can be explained by the Flory-Huggins model and since there is no convincing evidence to indicate strong specific solute-solvent interactions, the observed negative deviations from Raoult's law appears to be an artifact of the model caused by large molecular size disparity. The solubility measurements of Chiou and Manes, combined with an earlier study on glycerol trioleate/water partition coefficients (16), suggest that the Flory-Huggins model should be considered in systems having molar volume ratios of 4 or more.

#### SCATCHARD-HILDEBRAND SOLUBILITY PARAMETER THEORY

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

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

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

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

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

Comparison Between Experimental and Predicted Naphthalene Solubilities TABLE II.

olvent	$\delta_2^{\ a}$	v <sub>m,2</sub> a	x <sub>1</sub> (exp) <sup>b</sup>	$x_1(calc)$
ichloromethane	20.21	64.50	0.330	0.311
hlorobenzene	19.78	102.26	0.311	0.312
enzene	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
hylbenzene	18.08	123.08	0.289	0.289
etrachloromethane	17.49	97.08	0.255	0.275
clohexane	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

<sup>&</sup>lt;sup>a</sup>  $\delta_2/(10^3 \text{ g/kg}^{1/2} \text{ m}^{-1/2} \text{ s}^{-1}); V_{m,2}/(\text{cm}^3 \text{ mol}^{-1}).$ 

TABLE III. Comparison Between Experimental and Predicted Biphenyl Solubilities

Solvent	$\delta_2^{a}$	v <sub>m,2</sub> a	x <sub>1</sub> (exp) <sup>b</sup>	$x_1(calc)$
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

b Experimental solubilites were determined by Chang (63).

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

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

The popularity of the solubility parameter approach arises because it relates the solubility of a solute in a given solvent, either pure or mixed, to the bulk properties of the pure components. Whereas this particular application of the solubility parameter theory has certain practical advantages in that it requires only a minimal number of experimental observations, a more flexible expression for binary solvent systems can be derived by replacing the individual  $\delta_1$  values with the measured solubilities in the pure solvents and the measured thermodynamic excess properties of the solvent mixture.

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

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

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

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

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

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

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

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

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

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

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

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

#### MOBILE ORDER THEORY FOR BINARY ALKANE + ALCOHOL SOLVENT MIXTURES

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

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

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

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

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

The afore mentioned studies, along with many others too numerous to list, document the complexity of solutions containing a self-associating alcohol component, and the difficulty in developing an universal thermodynamic model applicable to all systems commonly encountered. During the past three decades many thermodynamic models have been suggested for both excess enthalpies and vapor-liquid equilibria for mixtures containing an alcohol with inert and with nonassociating active cosolvents. There has been little effort, however, devoted to developing descriptive models for crystalline solutes dissolved in alcoholic solvents. Scarcity of predictive methods for solid-liquid equilibria results, to a large extent, from the nature of solid solute

isothermal solubility measurements. There is only a single data point associated with the solubility of a crystalline solute in each neat organic solvent or solvent mixture, from which the solvent self-association equilibrium constant as well as all nonspecific interaction parameters and any solute-solvent association constants must be deduced.

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

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

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

In  $\phi_A$  = In  $a_A(s)$  - 0.5 (1 -  $V_{m,A}/V_{m,solvent}$ )  $\phi_{solvent}$  + 0.5 In  $[\phi_A^{sat} + \phi_{solvent}(V_A/V_{solvent})]$  -  $\phi_{solvent}^2$   $V_{m,A}(\delta_A' - \delta_{solvent}')^2$   $(RT)^{-1}$  -  $r_S$   $(V_{m,A}/V_{m,solvent})$   $\phi_{solvent}$  [26] where the  $r_S$   $(V_{m,A}/V_{m,solvent})$   $\phi_{solvent}$  term represents the contributions resulting from hydrogen-bond formation between the solvent molecules. For most of the published applications,  $r_S$  was assumed to be unity for strongly associated solvents with single hydrogen-bonded chains like alcohols, to be two for water or diols, and to equal zero for non-associated solvents such as saturated hydrocarbons. A more exact value for alcoholic solvents can be calculated based upon (46)

 $r_{S} = (K_{S} \phi_{solvent}/V_{m,solvent})/(1 + K_{S} \phi_{solvent}/V_{m,solvent})$  [27] with a numerical value of  $K_{S} = 5,000 \text{ cm}^{3} \text{ mol}^{-1}$  used for monofunctional alcohols.

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

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

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

 $<sup>^{\</sup>rm a}$  Tabulated values are taken from a compilation given in Ruelle et al. (47,48).

<sup>&</sup>lt;sup>b</sup> The numerical value of  $a_A(s) = 0.01049$  was calculated from the molar enthalpy of fusion,  $\Delta H^{fus}$ , at the normal melting point temperature of the solute,  $T_{MP} = 515$  K.

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

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

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

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

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

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

RT {ln [a<sub>A</sub>(s)/
$$\phi_A$$
] - 0.5[1- V<sub>m,A</sub>/( $x_B^{(s)}$ V<sub>m,B</sub> +  $x_C^{(s)}$ V<sub>m,C</sub>)] + 0.5 ln [V<sub>A</sub>/( $x_B^{o}$ V<sub>B</sub> +  $x_C^{o}$ V<sub>C</sub>)]

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

$$+ \phi_C^{(s)} (\delta_A^{i} - \delta_C^{i})^2 - \phi_B^{(s)} \phi_C^{(s)} (\delta_B^{i} - \delta_C^{i})^2]$$
[28]

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

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

and

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

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

$$\ln \phi_{A} = \phi_{B}^{(s)} \ln (\phi_{A})_{B} + \phi_{C}^{(s)} \ln (\phi_{A})_{C} - 0.5 \left[ \ln (x_{B}^{(s)}V_{m,B} + x_{C}^{(s)}V_{m,C}) - \phi_{B}^{(s)} \ln V_{m,B} \right]$$

$$- \phi_{C}^{(s)} \ln V_{m,C} + (V_{m,A} K_{C} \phi_{C}^{(s)}/V_{C}^{2}) (1 + K_{C}/V_{m,C})^{-1} - [V_{m,A} K_{C} \phi_{C}^{(s)2}/V_{m,C}^{2}] \times$$

$$(1 + \phi_{C}^{(s)} K_{C}/V_{m,C})^{-1} + V_{A} \phi_{B}^{(s)} \phi_{C}^{(s)} (\delta_{B}^{s} - \delta_{C}^{s})^{2} (RT)^{-1}$$

$$[31]$$

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

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

critically evaluate the measured solubility data for possible outliers.

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

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

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

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

<sup>&</sup>lt;sup>a</sup> Deviation (%) = (100/N)  $\Sigma$  | ln [x<sub>A</sub>(cal)/x<sub>A</sub>(exp)].

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

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

#### MOBILE ORDER THEORY FOR BINARY ALCOHOL + ALCOHOL SOLVENT MIXTURES

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

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

and

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

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

$$G = n_{A} \mu_{A}^{*} + n_{B} \mu_{B}^{*} + n_{C} \mu_{C}^{*} + n_{B} RT \ln \gamma_{B} + n_{C} RT \ln \gamma_{C} + 0.5 RT \{n_{A} \ln \phi_{A} + n_{B} \ln \phi_{B} + n_{C} \ln \phi_{C} + n_{A} \ln x_{A} + n_{B} \ln x_{B} + n_{C} \ln x_{C} \} + (n_{A}V_{m,A} + n_{B}V_{m,B} + n_{C}V_{m,C})$$

$$[\phi_{A} \phi_{B} (\delta_{A}^{'} - \delta_{B}^{'})^{2} + \phi_{A} \phi_{C} (\delta_{A}^{'} - \delta_{C}^{'})^{2} + \phi_{B} \phi_{C} (\delta_{B}^{'} - \delta_{C}^{'})^{2}]$$
[34]

and saturation solubility of a sparingly soluble solute

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

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

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

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

and

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

where  $(\phi_A^{\rm sat})_{\rm B}$  and  $(\phi_A^{\rm sat})_{\rm C}$  denote the solubilities in the two pure solvents. After

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

$$\ln \phi_{A} = \phi_{B}^{(s)} \ln (\phi_{A})_{B} + \phi_{C}^{(s)} \ln (\phi_{A})_{C} - 0.5 \left[ \ln (x_{B}^{(s)}V_{m,B} + x_{C}^{(s)}V_{m,C}) - \phi_{B}^{(s)} \ln V_{m,B} \right.$$

$$- \phi_{C}^{(s)} \ln V_{m,C} - (V_{m,A}/V_{m,B}) \phi_{B}^{(s)} \left[ \phi_{B}^{(s)} (K_{B}/V_{m,B}) + \phi_{C}^{(s)} (K_{BC}/V_{m,C}) \right]$$

$$+ \left[ 1 + \phi_{B}^{(s)} (K_{B}/V_{m,B}) + \phi_{C}^{(s)} (K_{BC}/V_{m,C}) \right] + (V_{m,A} K_{B} \phi_{B}^{(s)}/V_{m,B}^{2}) (1 + K_{B}/V_{m,B})^{-1}$$

$$- (V_{m,A}/V_{m,C}) \phi_{C}^{(s)} \left[ \phi_{B}^{(s)} (K_{CB}/V_{m,B}) + \phi_{C}^{(s)} (K_{C}/V_{m,C}) \right] / [1 + \phi_{B}^{(s)} (K_{CB}/V_{m,B})$$

$$+ \phi_{C}^{(s)} (K_{C}/V_{m,C}) \right] + (V_{m,A} K_{C} \phi_{C}^{(s)}/V_{m,C}^{2}) (1 + K_{C}/V_{m,C})^{-1}$$

$$+ V_{m,A} \phi_{B}^{(s)} \phi_{C}^{(s)} (\delta_{B}^{s} - \delta_{C}^{s})^{2} (RT)^{-1}$$

$$[38]$$

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

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

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

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

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

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

### MATHEMATICAL REPRESENTATION OF SOLUBILITY DATA IN BINARY SOLVENTS

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

$$(Z_{ABC}^{E})^{exp} - (Z_{ABC}^{E})^{calc} = x_A x_B x_C Q_{ABC}$$
 [39]

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

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

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

Conceptually, these ideas can be extended to solute solubilities in binary solvent mixtures, however, there has never been up until this volume a sufficiently large solid solute solubility data base to warrant computerized storage in equational form. With computerized data storage and retrieval becoming increasingly popular, it seems appropriate to review the various mathematical expressions that have been proposed in the chemical literature for describing the variation of solute solubility with binary solvent composition. Like the predictive expressions discussed in the

preceding sections, mathematical representations provide not only a means to screen experimental data sets for possible outliers in need of redetermination, but also facilitate interpolation at solvent compositions falling between measured data points.

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

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

or Modified Wilson equation

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

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

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

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

Solvent (B) + Solvent (C)	Λ <sub>, j</sub> adj,a	% Dev.b
t-Butylcyclohexane + 2,2,4-trimethylpentane	1.453	0.1
c-Butyleyelonexane + 2,2,4-trimethylpentame	0.981	0.1
	1.360	0.5
n-Hexane + 1-propanol	1.440	0.5
- Washing I I managed	1.440	0.7
n-Heptane + 1-propanol	1.410	0.7
- Oshawa   1 awarana)	1.240	0.6
n-Octane + 1-propanol	1.240	0.6
Cyclohexane + 1-propanol	1.300	1.6
Cyclonexane + 1-propanol	1.600	1.6
(abbulanalabanana 1.1 manana)		
Methylcyclohexane + 1-propanol	1.344	1.4
	1.667	
2,2,4-Trimethylpentane + 1-propanol	1.100	0.6
	1.500	
t-Butylcyclohexane + 1-propanol	1.225	1.0
	2.321	
n-Hexane + 2-propanol	1.409	0.7
	1.605	
n-Heptane + 2-propanol	0.962	0.6
	2.085	
n-Octane + 2-propanol	0.913	0.3
	2.365	
Cyclohexane + 2-propanol	1.657	0.5
	1.701	
Methylcyclohexane + 2-propanol	1.689	0.6
	1.801	
2,2,4-Trimethylpentane + 2-propanol	0.956	0.3
	1.797	
t-Butylcyclohexane + 2-propanol	1.378	1.4
	2.557	
n-Hexane + 1-butanol	1.690	0.4
	1.088	
n-Heptane + 1-butanol	1.476	0.5
	1.291	
n-Octane + 1-butanol	1.460	0.5
	1.500	
Cyclohexane + 1-butanol	2.377	0.5
-	1.010	
Methylcyclohexane + 1-butanol	2.387	0.9
	1.080	
2,2,4-Trimethylpentane + 1-butanol	2.600	1.8
	0.680	2.0
t-Butylcyclohexane + 1-butanol	1.525	0.7
	1.689	0.7
n-Hexane + 2-butanol	1.477	^ F
	1.481	0.5
n-Heptane + 2-butanol	1.481	
· supulser · & Allenda		0.3
n-Octane + 2-butanol	1.849	<b>.</b> .
* Occurs + T-Michial	0.949	0.4
	2.205	

TABLE VII. (Continued)		
Cyclohexane + 2-butanol	2.157	0.5
	1.345	
Methylcyclohexane + 2-butanol	1.885	0.6
	1.593	
2,2,4-Trimethylpentane + 2-butanol	1.097	0.4
• •	1.633	
-Butylcyclohexane + 2-butanol	1.325	0.5
	2.225	
n-Hexane + 1-octanol	2.501	0.6
	0.601	
n-Heptane + 1-octanol	2.201	0.3
. Hopeand . R wednes	0.685	
n-Octane + 1-octanol	1.901	0.2
1-occase + 1-occasor	0.801	
must shows a 1 askanol	4.733	0.4
Cyclohexane + 1-octanol	0,213	
water a contract to the same of the same o	9.568	0.2
Methylcyclohexane + 1-octanol	0.102	
	2.009	0.3
2,2,4-Trimethylpentane + 1-octanol	0.493	0.0
	3.097	0.3
t-Butylcyclohexane + 1-octanol	0.577	0.3
		0.6
n-Hexane + 2-methyl-1-propanol	1.557	0.6
	1.417	
n-Heptane + 2-methyl-1-propanol	1.265	0.5
-	1.721	
n-Octane + 2-methyl-1-propanol	1.141	0.5
	1.969	
Cyclohexane + 2-methyl-1-propanol	2.197	0.6
	1.249	
Methylcyclohexane + 2-methyl-1-propanol	1.961	0.9
ndenyzejezonezane z massa.	1.501	
2,2,4-Trimethylpentane + 2-methyl-1-propanol	1.133	0.9
2,2,4-Irimethylpentand / I money	1.525	
t-Butylcyclohexane + 2-methyl-1-propanol	1.345	0.5
t-Butylcyclonexane + 2-methyl 1 propense	2.017	
a Lubanal	1.709	0.3
n-Hexane + 3-methyl-1-butanol	1.149	
	1.437	0.3
n-Heptane + 3-methyl-1-butancl	1.341	0.5
_	1.477	0.2
n-Octane + 3-methyl-1-butanol	1.529	0.2
Cyclohexane + 3-methyl-1-butanol	2.449	0.3
	0.977	
Methylcyclohexane + 3-methyl-1-butanol	2.453	0.4
	1.061	
2,2,4-Trimethylpentane + 3-methyl-1-butanol	1.449	0.2
· ·	1.121	
t-Butylcyclohexane + 3-methyl-1-butanol	1.701	0.4
	1.561	
1-Butanol + 1-propanol	1.293	0.2
I-Ddcdior - I-brokensa	0.857	
0 Pure 1 1-propono!	0.953	0.5
2-Propanol + 1-propanol	1.073	

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

<sup>&</sup>lt;sup>a</sup> Adjustable parameters for the Modified Wilson equation are ordered as  $\Lambda_{\rm BC}^{\rm adj}$  and then  $\Lambda_{\rm CB}^{\rm adj}$ . <sup>b</sup> & Dev. = (100/N)  $\Sigma$  | ln [ $x_{\rm A}$ (cal)/ $x_{\rm A}$ (exp)] |.

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

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

	0.000	0.6	0.909	0.4
n-Octane + 1-butanol	0.933 - 0.033	0.6	- 0.014	0.4
	- 0.033		0.088	
	0.810	0.9	0.088	0.5
Cyclohexane + 1-butanol	0.336	0.5	0.741	4.5
	0.336		0.223	
	0.948	1.1	0.850	1.0
Methylcyclohexane + 1-butanol	0.282		0.146	4
	0.202		0.295	
2,2,4-Trimethylpentane + 1-butanol	0.576	0.5	0.536	0.3
2,2,4-II Interny I periodice . I December	0.121		0.151	
	• · • · • · · · · · · · · · · · · · · ·		0.142	
t-Butylcyclohexane + 1-butanol	1.134	1.2	1.039	0.4
c-BdfAlfActouexane . 1-pacquor	- 0.210		- 0.109	
			0.372	•
n-Hexane + 2-butanol	1.165	0.3		
	- 0.081			
n-Heptane + 2-butanol	1.225	0.2		
	- 0.292			
n-Octane + 2-butanol	1.458	1.3		
	- 0.618			
Cyclohexane + 2-butanol	1,260	0.6		
	0.206			
Methylcyclohexane + 2-butanol	1.447	1.2		
	- 0.009			
2,2,4-Trimethylpentane + 2-butanol	1.070	8.0		
· ·	- 0.213			
t-Butylcyclohexane + 2-butanol	1.718	1.7	1.588	0.3
	- 0.612		- 0.493	
			0.497	
n-Hexane + 1-octanol	0.748	1.9	0.607	0.8
	0.488		0.448	
			0.479	
n-Heptane + 1-octanol	0.488	0.6	0.442	0.3
	0.231		0.229	
			0.159	
n-Octane + 1-octanol	0.330	0.1		
	0.135	1.6	0.400	0.7
Cyclohexane + 1-octanol	0.518	1.0	0.358	0.7
	0.421		0.431	
	0.574	2.4	0.431	1.0
Methylcyclohexane + 1-octanol	0.574	2.4	0.549	1.0
	0.374		0.614	
2,2,4-Trimethylpentane + 1-octanol	0.469	0.3		
2,2,4-ItImethAlbancane + I-occanol	0.247			
t-Butylcyclohexane + 1-octanol	0.428	0.9		
F-Buchtchclousware + f-occaror	0.236	J		
n-Hexane + 2-methyl-1-propanol	1.267	1.2	1.177	0.5
	- 0.080		- 0.032	-
			0.322	

	1.356	1.1	1.284	0.7
n-Heptane + 2-methyl-1-propanol	- 0.350	1.1	- 0.301	
	- 0.050		0.266	
n-Octane + 2-methyl-1-propanol	1.540	1.4	1.422	0.4
1-Octane + 2-methyl I propunet	- 0.570		- 0.464	
			0.447	
Cyclohexane + 2-methyl-1-propanol	1.214	1.3	1.116	0.3
of croudward a manual a fact	0.148		0.172	
			0.341	
Methylcyclohexane +	1.462	1.8	1.342	0.6
2-methyl-1-propanol	- 0.070		0.121	
• · ·			0.430	
2,2,4-Trimethylpentane +	1.090	1.5	0.972	0.4
2-methyl-1-propanol	- 0.221		- 0.100	
			0.462	
t-Butylcyclohexane +	1.688	1.4	1.576	0.1
2-methyl-1-propanol	- 0.549		- 0.435	
			0.432	
n-Hexane + 3-methyl-1-butanol	0.857	0.8		
	0.186			
n-Heptane + 3-methyl-1-butanol	0.802	0.3		
	0.021			
n-Octane + 3-methyl-1-butanol	1.014	0.6		
	- 0.112 0.786	1.1		
Cyclohexane + 3-methyl-1-butanol	0.788	7.7		
a shall a huhamal	0.378	0.9		
Methylcyclohexane + 3-methyl-1-butanol	0.358	0.5		
	0.663	0.3		
2,2,4-Trimethylpentane +	0.005	0.0		
3-methyl-1-butanol	1.092	0.5		
t-Butylcyclohexane + 3-methyl-1-butanol	- 0.087			
1-Butanol + 1-propanol	0.117	0.3		
I-Butanoi + I-propamoi	0.015			
2-Propanol + 1-propanol	0.068	0.7		
Z-Propanor + 1-propanor	0.058			
2-Butanol + 1-propanol	0.000	0.3		
Z-Bucanoz / I propune	0.000			
1-Octanol + 1-propanol	1.025	1.2		
	- 0.575			
1-Butanol + 2-propanol	0.243	0.6		
• •	- 0.011			
2-Butanol + 2-propanol	0.097	0.1		
· · · · · · · · · · · · · · · · · · ·	- 0.013			
1-Octanol + 2-butanol	0.871	1.1		

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

#### REFERENCES

- Acree, W.E., Jr. Thermodynamic Properties of Nonelectrolyte Solutions. Academic Press, Inc., Orlando, FL, 1984.
- Grant, D.J.W.; Higuchi, T. Solubility Behavior of Organic Compounds. Wiley-Intersciece, New York, NY, 1990.
- Hildebrand, J.H.; Scott, R.L. The Solubility of Nonelectrolytes. Reinhold Publishing Corp., New York, NY, 1955.
- James, K.C. Solubility and Related Properties. Marcel Dekker, Inc., New York, NY, 1986.
- Prausnitz, J.M.; Lichtenthaler, R.N.; Gomes de Azevedo, E. Molecular Thermodynamics of Fluid Phase Equilibrium. Prentice-Hall, Englewood Cliffs, NJ, 1986.
- Shinoda, K. Principles of Solution and Solubility. Marcel Dekker, Inc., New York, NY, 1978.
- 7. Weimer, R.F.; Prausnitz, J.M. J. Chem. Phys. 1965, 42, 3643.
- 8. Choi, P.B.; McLaughlin, E. AICHE J. 1983, 29, 150.
- 9. Yalkowsky, S.H.; Valvani, S.C. J. Pharm. Sci. 1980, 69, 912.
- 10. Acree, W.E., Jr. Thermochim. Acta 1991, 189, 37.
- 11. Acree, W.E., Jr. Thermochim. Acta 1993, 219, 97.
- 12. Chickos, J.S.; Hesse, D.G.; Liebman, J.F. J. Org. Chem. 1990, 55, 3833.
- Chickos, J.S.; Braton, C.M.; Hesse, D.G.; Liebman, J.F. J. Org. Chem. <u>1991</u>, 56, 927.
- 14. Chickos, J.S.; Acree, W.E., Jr., unpublished calculations.
- 15. Chiou, C.T.; Manes, M. J. Chem. Soc., Faraday Trans. 1 1986, 82, 243.
- 16. Chiou, C.T. Environ. Sci. Technol. 1985, 19, 57.
- 17. Barton, A.F.M. Handbook of Solubility Parameters and Other Cohesion Parameters.

  CRC Press, Inc., Boca Raton, FL, 1983.
- 18. Hoy, K.L. J. Paint Technol. 1970, 42, 76.
- 19. Martin, A.; Newberger, J.; Adjei, A. J. Pharm. Sci. 1980, 69, 487.
- 20. Martin, A.; Wu, P.L.; Adjei, A.; Beerbower, A.; Prausnitz, J.M. J. Pharm. Sci. 1981, 70, 1260.
- 21. Adjei, A.; Newberger, J.; Martin, A. J. Pharm. Sci. 1980, 69, 659.
- Ochsner, A.B.; Belloto, R.J., Jr.; Sokoloski, T.D. J. Pharm. Sci. 1985, 74,
   132.
- 23. Acree, W.E., Jr.; McCargar, J.W.; Zvaigzne, A.I.; Teng, I.-L. Phys. Chem. Liq. 1991, 23, 27.
- 24. Acree, W.E., Jr.; Zvaigzne, A.I. Thermochim. Acta 1991, 178, 151.
- 25. Arnett, E.M.; Joris, L.; Mitchell, E.; Murty, T.S.S.R.; Gorrie, T.M.; Schleyer, P.v.R. J. Am. Chem. Soc. 1970, 92, 2365.
- 26. Duer, W.C.; Bertrand, G.L. J. Am. Chem. Soc. 1970, 92, 2587.
- Saluja, P.P.S.; Young, T.M.; Rodewald, R.F.; Fuchs, F.H.; Kohli, D.; Fuchs, R.
   J. Am. Chem. Soc. 1977, 99, 2949.
- 28. Bertrand, G.L. J. Phys. Chem. 1975, 79, 48.

- 29. McCargar, J.W.; Acree, W.E., Jr. Phys. Chem. Liq. 1987, 17, 123.
- 30. McCargar, J.W.; Acree, W.E., Jr. J. Pharm. Sci. 1987, 76, 572.
- 31. Acree, W.E., Jr.; McCargar, J.W. J. Pharm. Sci. 1987, 76, 575.
- 32. McCargar, J.W.; Acree, W.E., Jr. J. Solution Chem. 1988, 17, 1081.
- 33. Acree, W.E., Jr.; McCargar, J.W. J. Mol. Liq. 1988, 37, 251.
- 34. Pimental, G.C.; McClellan, A.L. The Hydrogen Bond. Freeman, San Fransisco, CA, 1960.
- 35. Van Ness, H.C.; van Winkle, J.; Richtol, H.H.; Hollinger, H.B. J. Phys Chem. 1967, 71, 1483.
- 36. Tucker, E.E.; Christian, S.D. J. Phys. Chem. 1977, 81, 1295.
- 37. Fletcher, A.H.; Heller, C.A. J. Phys. Chem. 1967, 71, 3742.
- 38. Fletcher, A.H.; Heller, C.A. J. Phys. Chem. 1968, 72, 1839.
- 39. Dixon, W.B. J. Phys. Chem. <u>1970</u>, 74, 1396.
- 40. Anderson, B.D.; Rytting, J.H.; Higuchi, T. Int. J. Pharm. 1978, 1, 15.
- 41. Anderson, B.D.; Rytting, J.H.; Higuchi, T. J. Am. Chem. Soc. 1979, 101, 5194.
- 42. Huyskens, P.L.; Siegel, G.G. Bull. Soc. Chim. Belg. 1988, 97, 821.
- 43. Huyskens, P.L.; Haulait-Pirson, M.C.; Brandts Buys, X.M. J. Coating Technol. 1985, 57, 57.
- 44. Huyskens, P.L.; Haulait-Pirson, M.C.; Van der Borght, X. Farbe Lack 1986, 92, 1145.
- 45. Siegel, G.G.; Huyskens, P.L.; Vanderheyden, G. Ber. Bunsenges. Phys. Chem. 1990, 94, 549.
- 46. Ruelle, P.; Rey-Mermet, C.; Buchmann, M.; Nam-Tran, H.; Kesselring, U.W.; Huyskens, P.L. Pharm. Res. 1991, 8, 840.
- 47. Ruelle, P.; Buchmann, M.; Nam-Tran, H.; Kesselring, U.W. Int. J. Pharm. 1992, 87, 47.
- 48. Ruelle, P.; Buchmann, M.; Nam-Tran. H.; Kesselring, U.W. *Pharm. Res.* 1992, 9, 788.
- 49. Ruelle, P.; Sarraf, E.; Kesselring, U.W. Int. J. Pharm. 1994, 104, 125.
- 50. Ruelle, P.; Buchmann, M.; Man-Tran, H.; Kesselring, U.W. J. Environ. Sci. Technol. 1993, 27, 266.
- 51. Huyskens, P.L.; Haulait-Pirson, M.C. J. Mol. Liq. 1985, 31, 135.
- 52. Gordon, L.J.; Scott, R.L. J. Am. Chem. Soc. 1952, 74, 4138.
- 53. Acree, W.E., Jr.; Rytting, J.H. J. Pharm. Sci. 1983, 72, 292.
- 54. Acree, W.E., Jr.; Zvaigzne, A.I. Fluid Phase Equilibr., in press.
- 55. Domanska, U. Fluid Phase Equilibr. 1990, 55, 125.
- 56. Domanska, U. Ind. Eng. Chem. Res. 1990, 29, 470.
- 57. Domanska, U. Pol. J. Chem. <u>1981</u>, 55, 1715.
- 58. Buchowski, H. Pol. J. Chem. 1979, 53, 1127.
- 59. Domanska, U. Ind. Eng. Chem. Res. <u>1987</u>, 26, 1153.
- 60. Domanska, U.; Hofman, T. J. Solution Chem. 1985, 14, 531.
- 61. Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. 1988, 17, 519.

62.	Sabbah, R.; Pemenzi, O. C. R. Acad. Sci. Paris, Ser. II 1993, 575.	
63.	Chang, W., Ph.D. Dissertation, North Dakota State University, 1909.	
	·	
1		
ļ		
ľ		
ļ		
1		
}		
İ		
}		
1		

# ACENAPHTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

### A. Saturated Hydrocarbons (including cycloalkanes)

n-octadecane cyclohexane decahydronaphthalene

### B. Alkenes

### C. Aromatic Hydrocarbons

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

### D. Esters

#### E. Ethers

# F. Haloalkanes and Haloaromatic Hydrocarbons

trichloromethane tetrachloromethane

### G. Alcohols

methanol
ethanol
1-propanol
1-octanol

### H. Ketones

### I. Miscellaneous Pure Solvents

pyridine
thiophene
1,2,3,5-tetranitrobenzene

# J. Binary Solvent Mixtures

	<b>MPONENTS:</b> 1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]  2) n-Octadecane; C <sub>18</sub> H <sub>38</sub> ; [593-45-3]			ORIGINAL MEASUREMENTS:  Djordjevic, N.M.  Thermochim. Acta 1991, 177, 109-118.			
(1) Acenaphth							
(2) n-Octadeo							
ARIABLES:		<del></del>	PREPARED BY	<u>(;</u>			
Temperature			W.E. Acres	e, Jr.			
EXPERIMENTAL 1	/ALUES			<del> </del>	· · · · · · · · · · · · · · · · · · ·		
T/K	<b>x</b> <sub>2</sub>	<i>*</i> 1	T/K	×2	× <sub>1</sub>		
352.4	0.3075	0.6925	363.5	0.0792	0.9208		
332.4							
	0.2410	0.7590					

#### METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter.

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

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

were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

#### SOURCE AND PURITY OF MATERIALS:

- (1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
- (2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.

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

ESTIMATED ERRORS:

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

### ESTIMATED ERRORS:

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		McLaughl:	McLaughlin, E.; Zainal, H.A.			
(2) Cyclohex	ane; C <sub>6</sub> H <sub>12</sub> ; []	.10-82-7]	J. Chem.	3854-3857.		
VARIABLES:	<del></del>	·····	PREPARED 1	BY:		
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL	VALUES					
r/K	x <sub>2</sub>	<b>x</b> <sub>1</sub>	T/K	<b>x</b> 2	<b>x</b> <sub>1</sub>	
308.7	0.9120	0.0880	330.2	0.7188	0.2812	
323.2	0.7923	0.2077	334.0	0.6547	0.3453	
		AUXILIA	RY INFORMATION	Ą		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	MATERIALS:	
thermometer.	-	and a precision	Teer	verwertung, w	Gesellschaft fur was passed over an th benzene as eluant.	
wixtures or	lixtures of known concentrations sealed					

COMPONENTS:			ORIGINAL N	MEASUREMENTS:		
	(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]		Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.			
(2) Cyclonexa	me; c <sub>6</sub> n <sub>12</sub> ; [.	110-82-7]	J. Chem.	Eng. Data 1	<u>1985</u> , 30, 403-409.	
VARIABLES:			PREPARED BY: W.E. Acree, Jr.			
Temperature						
EXPERIMENTAL V	ALUES					
T/K	<i>x</i> <sub>2</sub>	<i>×</i> 1	T/K	<i>x</i> <sub>2</sub>	$x_{\dagger}$	
303.35	0.9147	0.0853	329.95	0.7016	0.2984	
307.35	0.8969	0.1031	334.65	0.6303	0.3697	
312.05	0.8726	0.1274	339.85	0.5355	0.4645	
316.45	0.8435	0.1565	346.45	0.4008	0.5992	
320.95	0.8069	0.1931	354.45	0.2258	0.7742	
325.65	0.7579	0.2421				
		AUXILIARY	INFORMATION			
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
thermometer.		and a precision	(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.			
noting the ter	mperature at	which the last	ESTIMATED F	ERRORS:		
trace of solid	d sointe dis	appeared.	T/K: preci	ision <u>+</u> 0.1.		

COMPONENTS:	OMPONENTS: (1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]			MEASUREMENTS:		
(1) Acenapht				Coon, J.E.; Auwaerter, J.E.; McLaughlin, E		
(2) Decahydr (91-17-8	onaphthalene; ]	C <sub>10</sub> H <sub>18</sub> ;	Fluid Pha	<u>1989</u> , 44, 305-3	<u>1989</u> , <i>44</i> , 305-345.	
VARIABLES:		<del></del>	PREPARED B	Y:		
Temperature			W.E. Acre	e, Jr.		
EXPERIMENTAL	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	*2	<i>x</i> <sub>1</sub>	
300.7	0.8761	0.1239	327.8	0.6698	0.3302	
310.9	0.8127	0.1873	336.0	0.5523	0.4477	
318.7	0.7504	0.2496	348.3	0.3403	0.6597	

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

# SOURCE AND PURITY OF MATERIALS:

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

### ESTIMATED ERRORS:

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

COMPONENTS:			ORIGINAL MEASUREMENTS:					
<ul> <li>(1) Acenaphthene; C<sub>12</sub>H<sub>10</sub>; [83-32-9]</li> <li>(2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]</li> </ul>			Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.  J. Chem. Eng. Data 1985, 30, 403-409.					
VARIABLES:	ABLES:			PREPARED BY:				
Temperature			W.E. Acree, Jr.					
EXPERIMENTAL V	ALUES							
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<b>x</b> 2	<b>x</b> <sub>1</sub>			
306.55	0.7747	0.2253	335.95	0.4899	0.5101			
312.95	0.7276	0.2724	345.75	0.3502	0.6498			
319.85	0.6691	0.3309						
328.05	0.5842	0.4158						
		AUXILIARY	INFORMATION	,				
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND PURITY OF 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			<ul> <li>(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.</li> <li>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</li> </ul>					
	mperature at	which the last	ESTIMATED	ERRORS:				
trace of soli	.d solute dis	appeared.	T/K: prec x <sub>1</sub> : ± 0.00	ision ± 0.1.				

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]  VARIABLES: Temperature		McLaughlin, E.; Zainal, H.A.		
		J. Chem. Soc. <u>1959</u> , 863-867.		
		PREPARED BY:		
		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		L		
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>		
303.8	0.8185	0.1815		
314.6	0.7460	0.2540		
336.4	0.5269	0.4731		
342.6 0.4448		0.5552		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(1) Purity not specified, Gesellschaft fur Teerverwertung, passed over an alumina column with benzene eluant.		
		(2) "AnalaR", was dried over sodium wire and freshly distilled before use.		
noting the temperature trace of solid solute	e at which the last	ESTIMATED ERRORS:		
		$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003 (compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:								
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]  VARIABLES:			Speyers, C.L.  Am. J. Sci. 1902, 14, 293-302.  PREPARED BY:							
						Temperature		W.E. Acre	ee, Jr.	
						EXPERIMENTAL	VALUES			
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>					
273.2	0.9212	0.0788	314.8	0.7071	0.2929					
283.5	0.8924	0.1076	334.7	0.5492	0.4508					
297.3	0.8347	0.1653								
		AUXILIARY	INFORMATION	ī						
METHOD: APPARATUS/PROCEDURE		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			(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.							
minutes. Saturated solution was with- drawn through a coarse filter and anal- yzed by specific gravity. Author noted that evaporation to dryness and weighing		(2) Purity not given, Kahlbaum, was distilled before use.								
	was subject t		ESTIMATED	ERRORS:						
agcompositero.	•••			ision ± 0.1. (relative en	rror, compiler).					

(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2]		ORIGINAL MEASUREMENTS:  Coon, J.E.; Auwaerter, J.E.; McLaughlin, E			
					Fluid Pha
		VARIABLES:			PREPARED B
Temperature		W.E. Acre			
EXPERIMENTAL	VALUES				
T/K	<b>x</b> <sub>2</sub>	<i>*</i> 1	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>
308.1	0.7479	0.2521	343.7	0.3825	0.6175
312.6	0.7151	0.2849	351.9	0.2539	0.7461
322.2	0.6359	0.3641			
331.9	0.5305	0.4695			

# 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 noting the temperature at which the last trace of solid solute disappeared.

### SOURCE AND PURITY OF MATERIALS:

- (1) 99.2 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.
- 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:	
<ul> <li>(1) Acenaphthene; C<sub>12</sub>H<sub>10</sub>; [83-32-9]</li> <li>(2) 1,2-Dimethylbenzene; C<sub>8</sub>H<sub>10</sub>; [95-47-6]</li> </ul>		Kravchenko, V.M.; Pastukhova, I.S.  Zhur. Fiz. Khim. 1957, 31, 1802-1811.	
Temperature		W.E. Acree, Jr.	
IPERIMENTAL VALUES			
T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>	
247.2	1.000	0.000	
246.7	0.978	0.022	
246.2	0.956	0.044	
245.4	0.945	0.055	
253.3	0.935	0.065	
261.0	0.917	0.083	
271.2	0.886	0.114	
287.3	0.821	0.179	
302.2	0.739	0.261	
313.8	0.653	0.347	
324.7	0.564	0.436	
332.2	0.488	0.512	
342.7	0.362	0.638	
351.7	0.249	0.751	
359.6	0.136	0.864	
368.3	0.000	1.000	

#### 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:		ORIGINAL MEASUREMENTS:	
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) 1,2,4,5-Tetramethylbenzene; C <sub>10</sub> H <sub>14</sub> ; [95-93-2]		Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.	
		PREPARED BY:	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	<i>x</i> <sub>2</sub>	$x_1$	
352.2	1.000	0.000	
347.9	0.918	0.082	
344.3	0.856	0.146	
338.2	0.769	0.231	
332.1	0.689	0.311	
323.6	0.577	0.423	
324.6	0.562	0.438	
325.7	0.553	0.447	
328.2	0.525	0.475	
331.6	0.487	0.513	
338.9	0.410	0.590	
347.4	0.303	0.697	
354.5	0.207	0.793	
363.7	0.072	0.928	
368.3	0.000	1.000	
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:		ORIGINAL MEASUREMENTS:		
(1) Acenaphthene; C <sub>12</sub> H	i <sub>10</sub> ; [83-32-9]	Kravchenko, V.M.; Pastukhova, I.S.		
(2) Naphthalene; C <sub>10</sub> H <sub>8</sub> ; [91-20-3]  VARIABLES:  Temperature		Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811		
		PREPARED BY:		
		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	x <sub>2</sub>	<b>x</b> <sub>1</sub>		
353.2	1.000	0.000		
343.3	0.849	0.151		
334.1	0.718	0.282		
329.2	0.654	0.346		
325.0	0.604	0.396		
323.2	0.583	0.417		
327.0	0.541	0.459		
335.7	0.450	0.550		
344.7	0.344	0.656		
351.3	0.257	0.743		
361.8	0.107	0.893		
368.3	0.000	1.000		

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

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) 2-Methylnaphthalene; C <sub>11</sub> H <sub>10</sub> ; [91-57-6]  VARIABLES: Temperature		Kravchenko, V.M.; Pastukhova, I.S.	
		Zhur. Fiz. Khim. 1957, 31, 1802-1811.	
		PREPARED BY:	
		W.E. Acree, Jr.	
XPERIMENTAL V	ALUES		
T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>	
307	1.000	0.000	
300	0.901	0.099	
297	0.860	0.140	
292	0.807	0.193	
290	0.9	0.212	
293	0.773	0.227	
301	9 0.724	0.276	
309	0.681	0.319	
318	0.615	0.385	
328	0.524	0.476	
337	0.435	0.565	
345	0.320	0.680	
353	0.216	0.784	
358	0.148	0.852	
368	0.000	1.000	
	,		
		ARY INFORMATION	
	TUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
thermal analy	was determined using a rais method (described in K. Kravchenko, J. Phys. Chem	(1) Purity and chemical source were not specified in paper, was recrystallized before use.	
visual observ	9, 13, 133), supplemented by ations.	(2) Purity and chemical source were not specified in paper, was distilled before use.	
		ESTIMATED ERRORS:	

## COMPONENTS: ORIGINAL MEASUREMENTS: (1) Acenaphthene; C<sub>12</sub>H<sub>10</sub>; [83-32-9] Kravchenko, V.M.; Pastukhova, I.S. (2) 2,6-Dimethylnaphthalene; C12H12; Zhur. Fiz. Khim. 1957, 31, 1802-1811. [581-42-0] VARIABLES: PREPARED BY: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K ×2 *x*<sub>1</sub> 1.000 0.000 383.2 0.846 374.5 0.154 0.728 0.272 366.9 360.2 0.626 0.374 349.0 0.504 0.496 344.4 0.440 0.560 339.7 0.402 0.598 342.9 0.365 0.635 0.706 348.2 0.294 0.817 356.1 0.183 363.5 0.076 0.924 368.3 0.000 1.000 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Purity and chemical source were not specified in paper, was recrystallized 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 before use. (2) Purity and chemical source were not specified in paper, was recrystallized visual observations. before use.

ESTIMATED ERRORS:

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

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

#### ORIGINAL MEASUREMENTS: COMPONENTS: (1) Acenaphthene; C<sub>12</sub>H<sub>10</sub>; [83-32-9] Kravchenko, V.M.; Pastukhova, I.S. (2) 2,7-Dimethylnaphthalene; $C_{12}H_{12}$ ; [582-16-1] Zhur. Fiz. Khim. 1957, 31, 1802-1811. VARIABLES: PREPARED BY: Temperature W.E. Acree, Jr. EXPERIMENTAL VALUES T/K **x**<sub>1</sub> x<sub>2</sub> 0.000 370.2 1.000 0.096 0.904 364.4 361.0 0.858 0.142 354.4 0.756 0.244 0.350 347.3 0.650 340.2 0.555 0.445 0.496 0.504 335.3 0.469 0.531 333.9 0.551 0.449 334.8 0.580 0.420 338.7 0.348 0.652 344.3 0.786 352.9 0.214 0.900 360.7 0.100 1.000 368.3 0.000

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

### SOURCE AND PURITY OF MATERIALS:

- 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) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		Kravchenko, V.M.; Pastukhova, I.S.		
(2) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  VARIABLES:		Zhur. Fiz. Khim. 1957, 31, 1802-1811.		
				PREPARED BY:
		Temperature		W.E. Acree, Jr.
EXPERIMENTAL VALUES		<u> </u>		
T/K	× <sub>2</sub>	x <sub>1</sub>		
489.7	1.000	0.000		
477.2	0.822	0.178		
466.2	0.706	0.294		
456.2	0.590	0.410		
443.2	0.484	0.516		
434.2	0.397	0.603		
418.2	0.294	0.706		
402.5	0.216	0.784		
387.5	0.156	0.844		
368.2	0.104	0.896		
361.2	0.086	0.914		
362.7	0.071	0.929		
364.4	0.051	0.949		
368.3	0.000	1.000		
METHOD: APPARATUS/PROCE		INFORMATION SOURCE AND PURITY OF MATERIALS:		
Phase diagram was deter thermal analysis method detail in V.M. Kravcher U.S.S.R. 1939, 13, 13 visual observations.	rmined using a d (described in nko, J. Phys. Chem.	<ul><li>(1) Purity and chemical source were not specified in paper, was recrystallized before use.</li><li>(2) Purity and chemical source were not specified in paper, was recrystallized before use.</li></ul>		
		ESTIMATED ERRORS:		
		$T/K$ : precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		Kravchenko, V.M.; Pastukhova, I.S.	
(2) Phenanthrene; C <sub>14</sub>	H <sub>10</sub> ; [85-01-8]	Zhur. Fiz. Khim. 1957, 31, 1802-1811.  PREPARED BY:	
VARIABLES:			
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	<i>x</i> <sub>2</sub>	$\mathbf{x_1}$	
372.5	1.000	0.000	
357.4	0.801	0.199	
347.7	0.707	0.293	
338.7	0.614	0.386	i
329.0	0.508	0.492	
334.5	0.459	0.541	ĺ
339.1	0.401	0.599	
346.7	0.314	0.686	
355.0	0.204	0.796	
362.0	0.099	0.901	
368.3	0.000	1.000	

### 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) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) Fluorene; C <sub>16</sub> H <sub>10</sub> ; [86-73-7]  VARIABLES: Temperature		Kravchenko, V.M.; Pastukhova, I.S.  Zhur. Fiz. Khim. 1957, 31, 1802-1811.	
		W.E. Acree, Jr.	
		EXPERIMENTAL VALUES	
T/K	<b>x</b> <sub>2</sub>	x <sub>1</sub>	
387.2	1.000	0.000	
379.6	0.889	0.111	
367.9	0.746	0.254	
356.0	0.619	0.381	
348.1	0.528	0.472	
339.3	0.438	0.562	
337.8	0.418	0.582	
340.9	0.382	0.618	
348.2	0.293	0.707	
355.6	0.194	0.806	
361.7	0.103	0.897	
368.3	0.000	1.000	

### 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) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [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	<b>x</b> <sub>2</sub>	$x_1$	
528.2	1.000	0.000	
513.2	0.853	0.147	
500.2	0.722	0.278	
477.8	0.613	0.387	
471.5	0.501	0.499	
457.0	0.404	0.596	
437.4	0.296	0.704	
416.2	0.204	0.796	
378.5	0.101	0.899	
364.2	0.072	0.928	
366.4	0.034	0.966	
368.2	0.000	1.000	

### 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) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-	9] Kravchenko, V.M.; Pastukhova, I.S.
(2) Fluoranthene; C <sub>16</sub> H <sub>10</sub> ; [206-44	<b>)</b>
VARIABLES:	PREPARED BY:
Temperature	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
т/к	$\mathbf{x_1}$
383.2 1.00	0 0.000
368.8 0.81	5 0.185
363.4 0.75	2 0.248
350.7 0.60	6 0.394
340.8 0.49	2 0.508
335.0 0.43	8 0.562
335.3 0.42	9 0.571
339.4 0.38	8 0.612
348.2 0.29	3 0.707
358.1 0.16	3 0.837
362.3 0.09	2 0.908
368.3 0.00	0 1.000

# 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) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		Speyers, C.L.				
(2) Trichloromethane;	CHCl <sub>3</sub> ; [67-66-3]	Am. J. Sci. 1902, 14, 293-302.				
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL VALUES		-				
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>				
273.0	0.8728	0.1272				
284.4	0.8346	0.1654				
325.9	0.5783	0.4219				
	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		<ul> <li>(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.</li> <li>(2) Purity unknown, several sources listed, washed with water, sulfuric acid, dried over calcium chloride and distilled.</li> </ul>				
the residue was subject decomposition.		ESTIMATED ERRORS:  T/K: precision ± 0.1.  x <sub>1</sub> : ± 8 % (relative error, compiler).				

COMPONENTS: (1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]			ORIGINAL MEASUREMENTS:  McLaughlin, E.; Zainal, H.A.  J. Chem. Soc. 1960, 2485-2488.				
							(2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]
VARIABLES:							PREPARED I
Temperature	Temperature		W.E. Acree, Jr.				
EXPERIMENTAL '	VALUES						
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	x <sub>1</sub>		
303.2	0.8195	0.1805	325.2	0.6415	0.3585		
314.6	0.7373	0.2627					
318.6	0.7013	0.2987					
·		AUXILIARY	INFORMATION	ī			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer.			(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluan				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		dried	R grade, sou l over anhydr listilled bef	rce not given, was ous calcium chloride ore use.			
noting the to	emperature at	which the last	ESTIMATED	ERRORS:			
CLUCE OF BOX.	trace of solid solute disappeared.			T/K: precision + 0.1.			

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

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		Speyers, C.L.					
(2) Methanol; CH <sub>4</sub> O; [67-56-1]  VARIABLES:			Am. J. Sci. <u>1902</u> , 14, 293-302.				
			PREPARED I	BY:			
Temperature		W.E. Acree, Jr.					
EXPERIMENTAL '	VALUES		<del></del>	<del>-,</del>			
T/K	x <sub>2</sub>	$x_1$	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>		
273.2	0.9961	C 0039	319.2	0.9845	0.0155		
285.6	0.9962	0.0038	335.5	0.9754	0.0246		
303.9	0.9927	0.0073					
		AUXILIARY	INFORMATION	N	·		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	D PURITY OF M	IATERIALS:		
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30			(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.				
minutes. Saturated solution was with- drawn through a coarse filter and anal- yzed by specific gravity. Author noted that evaporation to dryness and weighing		(2) Marked "Acetonfrei", from Kahlbaum, dried over calcium oxide and distilled before use.					
the residue of	was subject t	o too much	ESTIMATED	ERRORS:			
2200mp0526101	•••			cision ± 0.1. (relative e	rror, compiler).		

COMPONENTS:  (1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]		ORIGINAL MEASUREMENTS:					
		Speyers, C.L.					
(2) Ethanol; C <sub>2</sub> H <sub>6</sub> O; [64-17-5]			Am. J. Se	Am. J. Sci. <u>1902</u> , 14, 293-302.			
VARIABLES:			PREPARED I	BY:			
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL V	LUES	<del></del>					
T/K	<b>x</b> <sub>2</sub>	<b>x</b> 1	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>		
273.2	0.9943	0.0057	323.0	0.9614	0.0386		
283.2	0.9916	0.0084	344.8	0.8706	0.1294		
303.5	0.9830	0.0170					
			ARY 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:

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

### ESTIMATED ERRORS:

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

						1
COMPONENTS:			ORIGINAL	MEASUREMENTS:		
(1) Acenapht	hene; C <sub>12</sub> H <sub>10</sub> ;	[83-32-9]	Speyers, C.L.			
(2) 1-Propan			Am. J. Sci. <u>1902</u> , 14, 293-302.  PREPARED BY:			
VARIABLES:						
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	<b>x</b> 2	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	<i>*</i> 1	
273.2	0.9912	0.0088	323.5	0.9563	0.0437	
283.7	0.9903	0.0097	346.6	0.801	0.199	
304.3	0.9812	0.0188				
		AUXILIARY	INFORMATIO	И		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing		(2) Puri	ized from ald t temperature ty not given,	Kahlbaum, was recreased to a melting of 93.5 °C.  Kahlbaum, was dried and distilled	-	
the residue	was subject t		ESTIMATED	ERRORS:		
decomposition	11.		T/K: pred	cision + 0.1.		

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

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9] (2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> 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.			
EXPERIMENTAL VALUES				
t/°C	(mol dm <sup>-3</sup> )			
25.0 0.29	561			
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:			
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).			

COMPONENTS:			ORIGINAL N	MEASUREMENTS:			
	hene; C <sub>12</sub> H <sub>10</sub> ;	f83-32-91	Choi, P.B.; McLaughlin, E.				
(2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]		Ind. Eng. Chem. Fundam. 1983, 22, 46-51.					
VARIABLES:	ARIABLES: Temperature		PREPARED F	BY:			
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL 1	VALUES						
T/K	<b>x</b> <sub>2</sub>	<i>*</i> 1	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>		
306.7	0.7898	0.2102	343.7	0.3890	0.6113		
320.0	0.6834	0.3166					
332.9	332.9 0.5408 0.4592						
337.5	0.4809	0.5191					
<del></del>		AUXILIARY	INFORMATION	ŧ			
METHOD: APPAR	ATUS/PROCEDUR	Œ	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			Kingo		rug Houses, United ystallized and then		
			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
		which the last	ESTIMATED	ERRORS:			
	trace of solid solute disappeared.			rision <u>+</u> 0.1.			

COMPONENTS:			ORIGINAL MEASUREMENTS:				
(1) Acenapht	hene; C <sub>12</sub> H <sub>10</sub> ;	[83-32-9]	Choi, P.B.; McLaughlin, E.				
(2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]  ARIABLES:		Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-51.					
		PREPARED I	37:				
Temperature			W.E. Acre	ee, Jr.			
EXPERIMENTAL	VALUES	<del></del>	l				
T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>×</i> 1		
307.3	0.7416	0.2584	344.8	0.3572	0.6428		
319.6	0.6458	0.3542					
328.4	0.5593	0.4407					
335.7	0.4776	0.5224					
		AUXILIARY	INFORMATION	ſ			
ETHOD: APPAR	ATUS/PROCEDUR	Œ	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath and a precision thermometer.		(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and the zone refined.					
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) Gold Compa	Label, 99.9+ uny, was used	%, Aldrich Chemical as received.		
noting the t	emperature at	which the last	ESTIMATED	ERRORS:			
	race of solid solute disappeared.						

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

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Acenaphthene; C <sub>12</sub> H	10; [83-32-9]	Shinomiya, C.				
(2) 1,2,3,5-Tetranitro C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>8</sub> ; [3698-53	obenzene; -1]	J. Chem. Soc. Japan <u>1940</u> , 15, 259-270.				
VARIABLES:		PREPARED BY:				
Temperature		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>				
399.2	1.000	0.000				
388.2	0.802	0.198				
382.2	0.706	0.296				
381.7	0.572	0.428				
383.2	0.470	0.530				
381.2	0.429	0.571				
372.2	0.290	0.710				
362.7	0.235	0.765				
348.2 0.118 361.7 0.099		0.882				
		0.901				
369.2	0.000	1.000				

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

AUXILIARY INFORMATION						
METHOD: APPARATUS/PROCEDURE 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).					

# ACRIDINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

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

cyclohexane decahydronaphthalene

- B. <u>Alkenes</u>
- 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. <u>Miscellaneous Pure Solvents</u>

pyridine thiophene

J. Binary Solvent Mixtures

		_			<del>_</del>	
COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Acridine; C <sub>13</sub> H <sub>9</sub> N; [260-94-6] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]  VARIABLES:  Temperature		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.				
		PREPARED BY:				
		W.E. Acre	ee, Jr.			
EXPERIMENTAL '	VALUES					
T/K	<b>x</b> 2	<b>x</b> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>	
309.3	0.9791	0.0209	353.3	0.7550	0.2450	
320.3	0.9697	0.0303	356.1	0.7029	0.2971	
330.9	0.9508	0.0492				
345.4	0.8931	0.1069				
		AUXILIARY	INFORMATION	4		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.			(1) 99 %, Kodak Chemical Company, Rochester New York, USA, was purified by vacuum sublimation to purity of 99.87 %.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the to		which the last	ESTIMATED	ERRORS:		
crace or sol	ra soince ais	ehheatan.	T/K: pred x <sub>1</sub> : ± 0.0	cision ± 0.1.		

COMPONENTS: (1) Acridine; C <sub>13</sub> H <sub>9</sub> N; [260-94-6]		ORIGINAL M	ORIGINAL MEASUREMENTS:  Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.					
		Coon, J.E						
(2) Decahydr [91-17-8	(2) Decahydronaphthalene; C <sub>10</sub> H <sub>18</sub> ; [91-17-8]  WARIABLES: Temperature		Fluid Pha	Fluid Phase Equilibr. 1989, 44, 305-345				
VARIABLES:			PREPARED BY: W.E. Acree, Jr.					
Temperature								
EXPERIMENTAL	VALUES							
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>			
306.0	0.9705	0.0295	354.7	0.6791	0.3209			
320.7	0.9537	0.0463	358.1	0.6037	0.3963			
335.0	0.9031	0.0969						
345.7	0.8150	0.1850						

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

### SOURCE AND PURITY OF MATERIALS:

- (1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to a purity of 99.87 %.
- (2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

#### ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:					
(1) Acridine; C <sub>13</sub> H <sub>9</sub> N; [260-94-6] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.					
VARIABLES: Temperature			PREPARED BY:				
			W.E. Acree, Jr.				
EXPERIMENTAL '	VALUES						
T/K	*2	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>		
296.3	0.8996	0.1004	330.3	0.7122	0.2878		
304.7	0.8680	0.1320	335.6	0.6559	0.3441		
317.2	0.8002	0.1998					
324.2	0.7587	0.2413					
		AUXILIAR	( INFORMATION	4			
METHOD: APPAR	ETHOD: 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			(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.  (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
						noting the temperature at which the last trace of solid solute disappeared.	
order of the sound disappeared.			$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003.				

COMPONENTS:			ORIGINAL MEASUREMENTS:					
(1) Acridine	(1) Acridine; C <sub>13</sub> H <sub>9</sub> N; [260-94-6]			Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.				
(2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2] VARIABLES: Temperature			Fluid Phase Equilibr. 1989, 44, 305-345.					
			PREPARED BY: W.E. Acree, Jr.					
								EXPERIMENTAL
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>			
305.2	0.8517	0.1483	331.3	0.6956	0.3044			
306.9	0.8409	0.1591	336.7	0.6537	0.3463			
316.3	0.8023	0.1977						
322.4	0.7608	0.2392						
		AUXILIARY	INFORMATION	1				
METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF M	ATERIALS:			
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			(1) 99 %, Kodak Chemical Company, Rochester New York, USA, was vacuum sublimed to a final purity of 99.87 %. (2) 99.6+ %, Aldrich Chemical Company, was					
			stored over molecular sieves to remove trace water.  ESTIMATED ERRORS:					
			T/K: precision + 0.1.					

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

COMPONENTS:			ORIGINAL MEASUREMENTS:					
(1) Acridine; C <sub>13</sub> H <sub>9</sub> N; [260-94-6] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.					
VARIABLES:	'ARIABLES:			PREPARED BY:				
Temperature			W.E. Acree, Jr.					
EXPERIMENTAL Y	VALUES							
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>			
301.7	0.8385	0.1615	339.1	0.5899	0.4101			
309.3	0.7986	0.2014	339.9	0.5616	0.4384			
322.9	0.7209	0.2791						
328.5	0.6600	0.3400						
		AUXILIARY	INFORMATION	ī				
METHOD: APPAR	ETHOD: 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 noting the temperature at which the last trace of solid solute disappeared.			<ul> <li>(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.</li> <li>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</li> </ul>					
			ESTIMATED ERRORS:					
			T/K: precision ± 0.1. x <sub>1</sub> : ± 0.0003.					

(1) Acridine; C <sub>13</sub> H <sub>9</sub> N; [260-94-6] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]  VARIABLES: Temperature			ORIGINAL MEASUREMENTS:				
			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
T/K	<b>x</b> <sub>2</sub>	$x_1$	T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>		
302.1	0.8203	0.1797	331.6	0.6497	0.3503		
304.1	0.8024	0.1976	337.9	0.6115	0.3885		
314.2	0.7563	0.2437					
325.0	0.7056	0.2944					
		AUXILIARY	INFORMATION	ī			
METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			<ul> <li>(1) 99 %, Kodak Chemical Company, Rochester New York, USA, was purified by vacuum sublimation to purity of 99.87 %.</li> <li>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</li> </ul>				
							noting the temperature at which the last trace of solid solute disappeared.
			$T/K$ : precision $\pm$ 0.1.				

# ESTIMATED ERRORS:

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

#### ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

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

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

### B. Alkenes

### C. Aromatic Hydrocarbons

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

### D. <u>Esters</u>

ethyl ethanoate butyl ethanoate dimethyl hexanedioate diethyl hexanedioate dibutyl oxalate

#### E. Ethers

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

# F. Haloalkanes and Haloaromatic Hydrocarbons

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

## G. Alcohols

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

## H. Ketones

2-propanone 2-butanone

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

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

## J. Binary\_Solvent Mixtures

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

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

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Acree, W.E., Jr.; Rytting, J.H.  J. Pharm Sci. <u>1983</u> , 72, 292-296.		
(2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]			
variables:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0 0.9987	0.001290		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:		
	T/K: ± 0.05. x <sub>1</sub> : ± 1 % (relative error).		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ;	[120-12-7]	Mahieu, J.		
(2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]		Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	*2 <sup>8</sup>	x <sub>1</sub> a		
25.0	0.99853	0.00150		
a computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.				
	AUXILIARY INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		

Constant temperature bath, thermometer,

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 weighted. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated

and a precision balance.

after solvent had evaporated.

## ESTIMATED ERRORS:

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

(1) Purity and source not given.

(2) Purity and source not given.

30				
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C14H10;	[120-12-7]	Acree, W.E., Jr.; Rytting, J.H.		
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]  VARIABLES:  T/K = 298		J. Pharm Sci. <u>1983</u> , 72, 292-296.		
		PREPARED BY: W.E. Acree, Jr.		
t/°C	<i>x</i> <sub>2</sub>	$x_1$		
25.0 0.9984		0.001571		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solve glass bottles and allow for several days at con Attainment of equilibri repetitive measurements	ed to equilibrate stant temperature. um verified by . Aliquots of sat-	(2) 99 %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves and distilled shortly before use.		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Lissi, E.A.; Abuin, E.B.	
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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	$c_1/(\text{mol dm}^{-3})$	
20.0	0.0040	

ESTIMATED ERRORS:

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

# METHOD: APPARATUS/PROCEDURE

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

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

metrically at 356 nm.

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.

	3		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Acree, W.E., Jr.; Rytting, J.H.		
(2) n-Octane; C <sub>8</sub> H <sub>18</sub> ; [111-65-9]	J. Pharm Sci. <u>1983</u> , 72, 292-296.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0 0.9982	0.001850		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 356 nm.	ESTIMATED ERRORS:		
	$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	McCargar, J.W.; Acree, W.E., Jr.		
(2) n-Hexadecane; C <sub>16</sub> H <sub>34</sub> ; [544-76-3]	J. Pharm. Sci. <u>1987</u> , 76, 572-574.		
variables:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0 0.9962	0.00380		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-	(2) 99 %, Aldrich Chemical Company, was used as received.		
chloromethane. Concentrations determined spectrophotometrically at 356 nm.	ESTIMATED ERRORS:		
	$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).		

COMPONENTS:			ORIGINAL I	MEASUREMENTS:	
(1) Anthrace	ne; C <sub>14</sub> H <sub>10</sub> ; [1	20-12-7]	Djordjevic, N.M.		
(2) n-Octadecane; C <sub>18</sub> H <sub>38</sub> ; [593-45-3]  VARIABLES:		Thermochim. Acta 1991, 177, 109-118.  PREPARED BY:			
					Temperature
EXPERIMENTAL	VALUES				
T/K	<b>x</b> <sub>2</sub>	$x_1$	T/K	* <sub>2</sub>	× <sub>1</sub>
466.5	0.4423	0.5577	477.5	0.2000	0.8000
468.0	0.4091	0.5909	478.5	0.1857	0.8143
472.6	0.3226	0.6774	480.8	0.1487	0.8513
477.0	0.2385	0.7615	483.0	0.0989	0.9011
-		AUXILIARY	INFORMATIO	N	
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		Compa		, Aldrich Chemical e, Wisconsin, USA, was	
			, Aldrich Cher um-distilled 1	mical Company, was before use.	
points of bi	nary mixtures	using a Perkin-	ESTIMATED	ERRORS:	
Elmer DSC-2 differential scanning calori- meter and scan rate of 5 K/min.		T/K: pred x <sub>1</sub> : ± 0.0	cision ± 0.3 1003 (compiler	(compiler).	

EIPERIMENTAL VALUES  t/°C	<b>x</b> <sub>2</sub>	$x_1$
EXPERIMENTAL VALUES		
T/K = 298		W.E. Acree, Jr.
VARIABLES:	<del></del>	PREPARED BY:
(2) Cyclonexane; C <sub>6</sub> n <sub>12</sub> ;	(110-82-7)	J. Pharm Sci. <u>1983</u> , 72, 292-296.
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]		
		Acree, W.E., Jr.; Rytting, J.H.
Components:		ORIGINAL MEASUREMENTS:

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

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

- (1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99.5 %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves and distilled shortly before use.

## ESTIMATED ERRORS:

COMPONENTS:	COMPONENTS:		ORIGINAL M	EASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]  VARIABLES:		McLaughli	n, E.	W.B.; Auwaerter, J.E.;	
		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL V	VALUES				,
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>
346.8	0.9905	0.0095	391.2	0.9625	0.0375
358.5	0.9857	0.0143	402.4	0.9500	0.0500
366.8	0.9810	0.0190			
378.3	0.9745	0.0255			
		AUXILIARY	INFORMATION	1	
METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		Milwa talli (2) Gold Compa	ukee, Wiscon zed from tol Label, 99.9+ nny, was used	Chemical Company, sin, USA, was recrysuene.  %, Aldrich Chemical as received.	
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED $T/K: prec   x_1: \pm 0.0$	ision ± 0.1.		

(2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.		
VARIABLES:	PREPARED BY:		
T/K = 313	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub> ª	ж <sub>1</sub> <sup>a</sup>		
40.0 0.9969	0.00306		
a computed by compiler from published so solubilities, which were expressed as w solute per 100 grams of solvent.  AUXILIARY			
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 temperature. Aliquots of saturatured solu-	(1) Purity and source not given. (2) Purity and source not given.		
tions transferred into tared containers			

ORIGINAL MEASUREMENTS:

Mahieu, J.

COMPONENTS:

(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]

34			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [1	.20-12-7]	Tucker, S.A.; Acree, W.E., Jr.	
(2) Methylcyclohexane; C <sub>7</sub> H <sub>14</sub> ; [108-87-2]		Phys. Chem. Liq. <u>1989</u> , 20, 31-38.	
VARIABLES:		PREPARED BY:	
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	
25.0	0.9984	0.00165	
<u> </u>	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDUR	Œ	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company was stored over mole- cular sieves and distilled shortly before use.	
Concentrations determined metrically at 356 nm.	l spectrophoto-	ESTIMATED ERRORS:	
		$T/K: \pm 0.05.$ $x_1: \pm 1 % (relative error).$	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Acree, W.E., Jr.; Rytting, J.H.		
(2) Cyclooctane; C <sub>8</sub> H <sub>16</sub> ; [292-64-8]	J. Pharm Sci. <u>1983</u> , 72, 292-296.		
variables:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°c x <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0 0.9977	0.002258		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 356 nm.	ESTIMATED ERRORS:		
	$T/K$ : $\pm 0.05$ . $x_1$ : $\pm 1$ % (relative error).		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]		Acree, W.E., Jr.; Rytting, J.H.		
(2) 2,2,4-Trimethylpen [540-84-1]	tane; C <sub>8</sub> H <sub>18</sub> ;	J. Pharm Sci. <u>1983</u> , 72, 292-296.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	x <sub>2</sub>	x <sub>1</sub>		
25.0	0.9989	0.001087		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature b thermometer, and an ul spectrophotometer.		(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) 99+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecu- lar sieves and distilled shortly before use.		
Concentrations determine metrically at 356 nm.		ESTIMATED ERRORS:		
		$T/K: \pm 0.05.$ $x_1: \pm 1 \% $ (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Anderson, B.D.		
(2) 2,2,4-Trimethylpentane; C <sub>8</sub> H <sub>18</sub> ; [540-84-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C	(mol dm <sup>-3</sup> )		
25.0 0.00	0660		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.		
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecu- lar sieves to remove trace water.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:		
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).		

36				
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]		Zvaigzne, A.I.; Acree, W.E., Jr.		
(2) t-Butylcyclohexane; [3178-22-1]	c <sub>10</sub> H <sub>20</sub> ;	J. Chem. Eng. Data 1994, 39, 117-118.		
VARIABLES:	-	PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	*2	× <sub>1</sub>		
25.0	0.9980	0.001978		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEI	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bathermometer, and an ult spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 determine metrically at 356 nm.	ned spectrophoto-	ESTIMATED ERRORS:		
		T/K: ± 0.05. x <sub>1</sub> : ± 1 % (relative error).		

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

COMPONENTS:			ORIGINAL M	EASUREMENTS:						
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) Decahydronaphthalene; C <sub>10</sub> H <sub>18</sub> ; [91-17-8]  VARIABLES:  Temperature		Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.  Fluid Phase Equilibr. 1989, 44, 305-345.  PREPARED BY:  W.E. Acree, Jr.								
					EXPERIMENTAL V	VALUES		ļ		
					T/K	x <sub>2</sub>	$x_1$	T/K	x2	<i>x</i> <sub>1</sub>
					323.6	0.9921	0.0079	362.9	0.9701	0.0299
327.1	0.9913	0.0087	385.6	0.9413	0.0587					
342.5	0.9849	0.0151								
351.0	0.9796	0.0204								
		AUXILIARY	INFORMATION	ſ						
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:					
thermometer.			(1) 99.99 wauke recei	e, Wisconsin	Chemical Company, Mil- , USA, was used as					
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		isome	r ratio of 6	emical Company, having 0.6 % cis and 39.4 % r molecular sieves.						
noting the te	emperature at	which the last	T/K: prec	ision ± 0.1.						

Components:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]		Acree, W.E., Jr.; Rytting, J.H.			
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [7	1-43-2]	J. Pharm Sci. <u>1983</u> , 72, 292-296.		J. Pharm Sci. <u>1983</u> , 72, 292-296.	
VARIABLES:		PREPARED BY:			
r/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/°C	* <sub>2</sub>	x <sub>1</sub>			
25.0 0.9926		0.007418			
	AUXIL	IARY INFORMATION			

### AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

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

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

## SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) Spectroanalyzed, 99.9+ %, Fisher Chemical Company, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.

## ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Smutek, M.; Fris, M.; Fohl, J.
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; {71-43-2}	Collection Czech. Chem. Commun. 1967, 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 293 and 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	x <sub>1</sub>
20.0 0.9940	0.00595
25.0 0.9929	0.00711
AU	IXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE  Constant temperature bath, thermomet and a precision balance.  Excess solute and solvent placed in glass container and allowed to equil for several hours at constant temper Aliquots of saturated solutions were transferred into tared constainers a weighed. Solubilities calculated fr weight of solid residue that remaine after solvent had evaporated.	closed cl
	$T/K$ : precision $\pm$ 0.05. $x_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]  VARIABLES:		ORIGINAL MEASUREMENTS: Somayajulu, G.R.; Palit, S.R.				
						J. Phys. Chem. <u>1954</u> , 58, 417-421.  PREPARED BY:
		Temperature		W.E. Acre	ee, Jr.	
		EXPERIMENTAL '	VALUES			
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>	
305.2	0.9909	0.00912	320.2	0.9856	0.01437	
310.2	0.9894	0.01059	325.2	0.9830	0.01698	
315.2	0.9875	0.01245	330.2	0.9807	0.01934	
			340.2	0.9744	0.02558	
		AUXILIARY	INFORMATION	4		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE ANI	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant			<ol> <li>Purity not specified, J. T. Baker, USF was recrystallized several times from ethanol and ethyl ethanoate. tallized from toluene.</li> <li>AR Grade, thiophene free, source not specified, was dried over calcium chloride and distilled before use.</li> </ol>			
temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by						
trace of soli	id solute dis	which the last appeared. Reporvariation of mole temperature.		errors: cision ± 0.3. 0001 (compil	ier).	

## ESTIMATED ERRORS:

						3
COMPONENTS:			ORIGINAL MEASUREMENTS:  Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]		J.E.;				
			J. Solution Chem. <u>1988</u> , 16, 519-534.			
VARIABLES: Temperature		PREPARED BY: W.E. Acree, Jr.				
EXPERIMENTAL V	<b>VALUES</b>		ļ			
T/K	<b>x</b> <sub>2</sub>	× <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	
308.9	0.9899	0.0101	353.9	0.9607	0.0393	
330.6	0.9797	0.0203	364.3	0.9501	0.0499	
338.2	0.9743	0.0257				1
344.6	0.9697	0.0303				
		AUXILIARY	INFORMATION	Ī		
METHOD: APPARA	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.			Milwa		Chemical Company, sin, USA, was recr uene.	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by				%, Aldrich Chemic as received.	al	
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
trace of solid solute disappeared.		T/K: prec x <sub>1</sub> : ± 0.00	ision ± 0.1.			

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Mahieu, J.		
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	Bull. Soc. Chim. Belgique 1936, 45, 667-677.		
/ARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub> a	x <sub>1</sub> °		
25.0 0.9926	0.00740		
<sup>a</sup> computed by compiler from published so solubilities, which were expressed as we	olvent compositions and solute sight percent and grams of		
solubilities, which were expressed as we solute per 100 grams of solvent.	olvent compositions and solute eight percent and grams of INFORMATION		
solubilities, which were expressed as we solute per 100 grams of solvent.	eight percent and grams of		
solubilities, which were expressed as we solute per 100 grams of solvent.  AUXILIARY	eight percent and grams of INFORMATION		

ORIGINAL MEASUREMENTS:

### COMPONENTS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

### **EVALUATOR:**

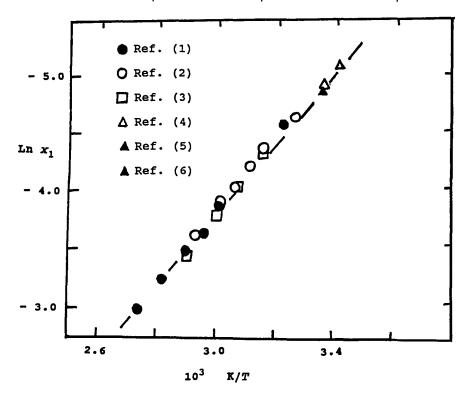
W.E. Acree, Jr.
Department of Chemistry
University of North Texas Denton, Texas June, 1994 76203-5068 (USA)

### CRITICAL EVALUATION:

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

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

 $Ln x_1 = -3200.1 (1/T) + 5.7899$ (r = 0.9987) nr >for variation of anthracene solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is  $x_1 = 0.00713$ , and differs by less than 4 % from experimental values of  $x_1 = 0.00711$  (4),  $x_1 = 0.007418$  (5) and  $x_1 = 0.00740$  (6).



Graphical plot of Ln  $x_1$  versus 1/T

## REFERENCES

- Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. J. Solution Chem. 1988, 16, 519-534.

  Somayajulu, G.R.; Palit, S.R. J. Phys. Chem. 1954, 58, 417-421.

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

  Smutek, M.; Fris, M.; Fohl, J. Coll. Czech. Chem. Commun. 1967, 32, 931-943. Acree, W.E., Jr.; Rytting, J.H. J. Pharm. Sci. 1983, 72, 292-296.

  Mahieu, J. Bull. Soc. Chim. Belgique 1936, 45, 667-677. 1.
- 2.
- з.
- 4.

COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]			ORIGINAL MEASUREMENTS:  McLaughlin, E.; Zainal, H.A.  J. Chem. Soc. 1959, 863-867.  PREPARED BY:  W.E. Acree, Jr.							
						(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]  VARIABLES:  Temperature				
EXPERIMENTAL V	VALUES							ļ <u> </u>		
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>						T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>
309.0	0.9897	0.0103				343.4	0.9685	0.0315		
315.6	0.9870	0.0130								
323.8	0.9827	0.0173								
332.8	0.9775	0.0225								
		AUXILIARY	INFORMATION	ī						
METHOD: APPARI	ATUS/PROCEDUR	Е	SOURCE AND	PURITY OF M	ATERIALS:					
Constant temp	perature bath	and a precision	(1) Purity, source and purification procedure not specified.							
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(2) "AnalaR", was dried over sodium wire and freshly distilled before use.							
noting the te	emperature at	which the last		ERRORS: ision ± 0.1. 003 (compiler						

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]		Tucker, S.A.; Murral, D.J.; Oswalt, B.M.; Halmi, J.L.; Acree, W.E., Jr.  Phys. Chem. Liq. 1988, 18, 279-286.		
VARIABLES:		PREPARED BY: W.E. Acree, Jr.		
r/K = 298				
EXPERIMENTAL VALUES				
t/°C	<b>x</b> <sub>2</sub>	$x_1$		
25.0	0.9926	0.00736		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature I thermometer, and an use spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.		(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use		
		ESTIMATED ERRORS:		

46					
Components:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]		Smutek,	M.; Fris, M.;	Fohl, J.	
(2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]		Collection Czech. Chem. Commun. 1967, 32, 931-943.			
VARIABLES:			PREPARED	BY:	
T/K = 293,	313 and 333		W.E. Acr	ee, Jr.	
EXPERIMENTAL	VALUES		ļ		
t/°C	<i>x</i> <sub>2</sub>	<b>×</b> 1	t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>
20.0	0.9935	0.00645	60.0	0.9770	0.0230
40.0	0.9876	0.0124			
		AUXILIARY	INFORMATIO	N	
METHOD: APPAR	ATUS/PROCEDUR	RE	SOURCE AN	D PURITY OF M	ATERIALS:
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.		Czec time to g	h., was recry s from pyridi ive a final p , Commercial	ty, Urxovy Zavady, stallized several ne and cyclohexane urity of 98.3 %. sample, source and od was not specified	
		ESTIMATED	ERRORS:		
		T/K: pred x <sub>1</sub> : ± 3 %	cision $\pm$ 0.05 (relative ex	. rror; compiler).	

METHOD: APPARATUS/PROCED	JRE	SOURCE AND PURITY OF MATERIALS:		
	AUXIL	IARY INFORMATION		
25.0	0.9927	0.00733		
t/°C	*2	<i>x</i> <sub>1</sub>		
EXPERIMENTAL VALUES				
T/K = 298		W.E. Acree, Jr.		
VARIABLES:		Phys. Chem. Liq. <u>1989</u> , 20, 31-38.  PREPARED BY:		
(2) 1,4-Dimethylbenzene [106-42-3]	; C <sub>8</sub> H <sub>10</sub> ;			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ;	[120-12-7]	Tucker, S.A.; Acree, W.E., Jr.		
COMPONENTS:		ORIGINAL MEASUREMENTS:		

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

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

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.5+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

## ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-	Smutek, M.; Fris, M.; Fohl, J.
(2) 1,4-Dimethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [106-42-3]	Collection Czech. Chem. Commun., <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	<b>x</b> <sub>1</sub>
25.0 0.9	923 0.00770
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, ther and a precision balance.  Excess solute and solvent place glass container and allowed to for several hours at constant taliquots of saturated solutions transferred into tared constain weighed. Solubilities calculated	Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.  equilibrate emperature. (2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that re	aained

COMPONENTS:		ORIGINAL MEASUREMENTS:				
<ul> <li>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</li> <li>(2) 4-Isopropyl methylbenzene; C<sub>10</sub>H<sub>14</sub>; [99-87-6]</li> </ul>		Wheeler, A.S.  J. Am. Chem. Soc. <u>1920</u> , 42, 1842-1846.				
					VARIABLES:	<del></del> _
Temperature		W.E. Acre	ee, Jr.			
EXPERIMENTAL	VALUES		ļ			
T/K	<b>x</b> <sub>2</sub>	<i>*</i> 1	T/K	* <sub>2</sub>	<i>*</i> 1	
298.2	0.9883	0.0117	373.2	0.9349	0.0651	
303.2	0.9872	0.0128				
		AUXILIARY	INFORMATION			
METHOD: APPAR	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 temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubilities calculated from weight of solid residue which remained after solvent had evaporated.			<pre>(1) Purity and source not given. (2) Purity and source not given.  ESTIMATED ERRORS:  T/K: precision ± 0.5 (compiler). x<sub>1</sub>: ± 5 % (relative error; compiler).</pre>			

COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS:		
		Kravchenko, V.M.; Pastukhova, I.S.		
		Zhur. Fiz. Khim. <u>1957</u> , 31, 1802-1811.		
		PREPARED BY: W.E. Acree, Jr.		
				EXPERIMENTAL VALUES
T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>		
368.3	1.000	0.000		
364.4	0.949	0.051		
362.7	0.929	0.071		
361.2	0.914	0.086		
368.2	0.896	0.104		
387.5	0.844	0.156		
402.5	0.784	0.216		
418.2	0.706	0.294		
434.2	0.603	0.397		
443.2	0.516	0.484		
456.2	0.410	0.590		
466.2	0.294	0.706		
477.2	0.178	0.822		
489.7	0.000	1.000		
METHOD: APPARATUS/PROCE		SOURCE AND PURITY OF MATERIALS:		
·				
Phase diagram was dete thermal analysis metho	d (described in	(1) Purity and chemical source were not specified in paper, was recrystallized before use		

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 recrystallized before use.

## ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]		Kravchenko, V.M.; Pastukhova, I.S.  Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	<b>x</b> <sub>2</sub>	<sup>x</sup> 1	
528.2	1.000	0.000	
519.2	0.896	0.104	
509.5	0.788	0.212	
499.7	0.693	0.307	
490.9	0.603	0.397	
480.4	0.496	0.504	
470.5	0.402	0.598	
466.2	0.365	0.635	
467.2	0.303	0.697	
469.7	0.260	0.740	
473.7	0.202	0.798	
481.7	0.103	0.897	
489.7	0.000	1.000	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:	
Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. 1939, 13, 133), supplemented by visual observations.		(1) Purity and chemical source were not specified in paper, was recrystallized before use.  (2) Purity and chemical source were not specified in paper, was recrystallized	
		before use.	
		<pre>ESTIMATED ERRORS:  T/K: precision ± 0.2 (Compiler). x<sub>1</sub>: ± 0.002 (Compiler).</pre>	

COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) Fluoranthene; C <sub>16</sub> H <sub>10</sub> ; [206-44-0]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS:  Kravchenko, V.M.; Pastukhova, I.S.		
		PREPARED BY:		
		W.E. Acree, Jr.		
		EXPERIMENTAL VALUES		
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>		
383.2	1.000	0.000		
377.8	0.930	0.070		
376.5	0.906	0.094		
375.0	0.884	0.116		
374.2	0.860	0.140		
380.2	0.859	0.141		
387.3	0.830	0.170		
395.7	0.804	0.196		
419.9	0.671	0.329		
435.2	0.566	0.434		
449.4	0.456	0.544		
459.7	0.355	0.645		
467.4	0.269	0.731		
475.1	0.178	0.822		
489.7	0.000	1.000		
		RY INFORMATION		
METHOD: APPARATUS/PROCE		SOURCE AND PURITY OF MATERIALS:		
Phase diagram was determal analysis methodetail in V.M. Kravche U.S.S.R. 1939, 13, 13	od (described in enko, J. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.		
visual observations.	,, sappromented by	(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
		ESTIMATED ERRORS:		
		$T/K$ : precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]			Coon, J.E	.; Auwaerter	, J.E.; McLaughlin, E.
(2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2]		Fluid Phase Equilibr. 1989, 44, 305-345.			
VARIABLES:			PREPARED F	BY:	
Temperature			W.E. Acre	ee, Jr.	
EXPERIMENTAL V	VALUES				
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>
299.6	0.9900	0.0100	343.4	0.9592	0.0408
319.5	0.9801	0.0199	346.2	0.9567	0.0433
327.6	0.9741	0.0259			
333.0	0.9697	0.0303			
		AUXILIARY	INFORMATION	T	
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last				e, Wisconsin	Chemical Company, Mil- , USA, was used as
			store		Chemical Company, was ular sieves to remove
			ESTIMATED	ERRORS:	
trace of solid solute disappeared.		T/K: pred x <sub>1</sub> : ± 0.0	ision <u>+</u> 0.1.		

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120	1-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.  Phys. Chem. Liq. 1991, 24, 31-42.  PREPARED BY:		
(2) Ethyl ethanoate; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> . [141-78-6]	•			
VARIABLES:	····			
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	<b>x</b> <sub>2</sub>	× <sub>1</sub>		
25.0	0.9952	0.00484		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and an ultravispectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent programs of the several days at constant Attainment of equilibrium repetitive measurements. Alturated solutions transferre coarse filter into tared voflasks, weighed and diluted	to equilibrate temperature. erified by iquots of sat- d through a blumetric	(2) 99.5+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.		
Concentrations determined a metrically at 356 nm.	pectrophoto-	ESTIMATED ERRORS:		
		T/K: ± 0.05. x;: ± 1.5 % (relative error).		

ORIGINAL MEASUREMENTS:

40				
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ;	; [120-12-7]	Acree, W.E., Jr.		
(2) Butyl ethanoate; ( [123-86-4]	<sup>5</sup> 6 <sup>H</sup> 12 <sup>O</sup> 2;	J. Chem. Soc. Faraday Trans. <u>1991</u> , 87, 461-464.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	× <sub>2</sub>	× <sub>1</sub>		
25.0	0.9934	0.00661		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	EDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature I thermometer, and an use spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 determmetrically at 356 nm.	ined spectrophoto-	ESTIMATED ERRORS:		
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).		

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Dimethyl hexanedioate; C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> ; [627-93-0]		Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr.  Phys. Chem. Liq. 1992, 25, 51-58.	
VARIABLES:		PREPARED BY:	
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	* <sub>2</sub>	<i>×</i> 1	
25.0	0.9913	0.00871	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature be thermometer, and an ul spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solve glass bottles and allow for several days at containment of equilibrary repetitive measurement urated solutions transcoarse filter into tar flasks, weighed and di	wed to equilibrate instant temperature. ium verified by s. Aliquots of sat-ferred through a ed volumetric	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.	
flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.		ESTIMATED ERRORS:	
		T/K: ± 0.05.	

		48
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ;	[120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) Diethyl hexanedioa [141-28-6]	te; C <sub>10</sub> H <sub>18</sub> O <sub>4</sub> ;	Phys. Chem. Liq. <u>1991</u> , 24, 31-42.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>
25.0	0.9897	0.01033
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature be thermometer, and an ul spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solve glass bottles and allowed for several days at concept and the several days at the several days and the several days and the several days are several days and the several days are several days and the several days and the several days are several days at the several days are several days at the sev	wed to equilibrate nstant temperature. ium verified by s. Aliquots of satferred through a ed volumetric luted with methanol.	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.
Concentrations determine metrically at 356 nm.	ned spectrophoto-	ESTIMATED ERRORS:
<u> </u>		$T/K: \pm 0.05.$ $x_1: \pm 1.5 \%$ (relative error).

COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) Dibutyl Oxalate; C <sub>10</sub> H <sub>18</sub> O <sub>4</sub> ;  [2050-60-4]  VARIABLES:  T/K = 298		ORIGINAL MEASUREMENTS:  Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr.  Phys. Chem. Liq. 1992, 25, 51-58.  PREPARED BY:  W.E. Acree, Jr.			
			EXPERIMENTAL VALUES		
			t/°C	<b>x</b> <sub>2</sub>	× <sub>1</sub>
			25.0	0.9896	0.01043
	AUXILIAR	Y INFORMATION			
METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.			

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a

flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

coarse filter into tared volumetric

## ESTIMATED ERRORS:

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

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

ORIGINAL MEASUREMENTS:
OKIGINAL MEASUREMENTS:
Mahieu, J.
Bull. Soc. Chim. Belgique 1936, 45, 667-677.
PREPARED BY:
W.E. Acree, Jr.
<i>x</i> <sub>1</sub> <sup>a</sup>
0.00353
olvent compositions and solute eight percent and grams of
INFORMATION
SOURCE AND PURITY OF MATERIALS:
(1) Purity and source not given.
(2) Purity and source not given.
TOTAL
ESTIMATED ERRORS:
$T/K$ : precision $\pm$ 0.5 (compiler). $x_1$ : $\pm$ 5 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Marthandan, M.V.; Acree, W.E., Jr.
(2) 1,1-Oxybisbutane; C <sub>8</sub> H <sub>18</sub> O; [142-96-1]	J. Chem. Eng. Data 1987, 32, 301-303.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>
25.0 0.996	4 0.003609
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorithermometer, and an ultraviolet/v spectrophotometer.	metric (1) Gold Label, 99.9 %, Aldrich Chemical company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed glass bottles and allowed to equi for several days at constant temp. Attainment of equilibrium verifier repetitive measurements. Aliquots urated solutions transferred throcoarse filter into tared volumetr flasks, weighed and diluted with the second	librate company, was stored over molecular erature. sieves and distilled shortly before use. do by of sature ugh a cic merhanol.
Concentrations determined spectrometrically at 356 nm.	photo- ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).

		J			
COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) 1,1-Oxybisbutane; C <sub>8</sub> H <sub>18</sub> O; [142-96-1]		ORIGINAL MEASUREMENTS:  McCargar, J.W.; Acree, W.E., Jr.  J. Pharm. Sci. 1987, 76, 572-574.			
			VARIABLES:		PREPARED BY:
			T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES					
±/°C	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>			
25.0	0.9965	0.00354			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	EDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-		(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.			
chloromethane. Concer spectrophotometrically		ESTIMATED ERRORS:			
		T/K: ± 0.05. x <sub>1</sub> : ± 1 % (relative error).			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Anderson, B.D.
(2) 1,1-Oxybisbutane; C <sub>8</sub> H <sub>18</sub> O; [142-96-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
25.0 0.0	210
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received.
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).

52		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
(2) Tetrahydrofuran; C <sub>4</sub> H <sub>8</sub> O; [109-99-9]		
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub> x <sub>1</sub>		
0.991 0.0	09	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).	

AUXILIARY INFORMATION		
25.0	0.9898	0.01024
t/°C	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>
EIPERIMENTAL VALUES		
T/K = 298		W.E. Acree, Jr.
ARIABLES:		Bissell, M.; Chittick, C.E.; Acree, W.E., Jr.  Fluid Phase Equilibr. 1988, 41, 187-194.  PREPARED BY:
<ol> <li>Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</li> <li>Tetrahydropyran; C<sub>5</sub>H<sub>10</sub>O; [142-68-7]</li> </ol>		
COMPONENTS:		ORIGINAL MEASUREMENTS:

# METHOD: APPARATUS/PROCEDURE

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

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

## SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company was stored over molecular sieves and distilled shortly before use.

## ESTIMATED ERRORS:

# COMPONENTS: ORIGINAL MEASUREMENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation) (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-17-7] (2) 1,4-Dioxane; C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>; [123-91-1] VARIABLES: PREPARED BY: T/K = See belowW.E. Acree, Jr. EXPERIMENTAL VALUES x<sub>2</sub> ×<sub>1</sub> 0.9904 0.0096 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: No experimental details were given in (1) Purity and chemical source not specithe paper. fied in paper. (2) Purity and chemical source not speci-fied in paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K. **ESTIMATED ERRORS:**

T/K: Unknown.

ORIGINAL MEASUREMENTS:

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

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 1,4-Dioxane; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ; [123-91-1] VARIABLES: T/K = 298			Procyk, A.D.; Bissell, M.; Street, K.W., Jr.; Acree, W.E., Jr.  J. Pharm. Sci. 1987, 76, 621-626.  PREPARED BY:  W.E. Acree, Jr.	
EXPERIMEN	ITAL VALUES			
	t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	
	25.0	0.9916	0.008381	
	<del> </del>	AUXILIARY	INFORMATION	
METHOD: A	APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:	
thermome		bath, calorimetric ltraviolet/visible	(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.		owed to equilibrate onstant temperature. rium verified by ts. Aliquots of satserred through a red volumetric	(2) HPLC Grade, 99.8 %, 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).	

)4	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.
(2) 1,4-Dioxane; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ; [123-91-1]	Environ. Sci. Technol. <u>1990</u> , 24, 639-646.
VARIABLES:	PREPARED BY:
T/K = 296	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
23.0 0.0	756
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:
	$T/K$ : $\pm$ 1. $c_1$ : $\pm$ 5% (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7	Smutek, M.; Fris, M.; Fohl, J.
(2) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	Collection Czech. Chem. Commun. 1967, 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	× <sub>1</sub>
25.0 0.98	395 0.0105
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermand a precision balance.  Excess solute and solvent placed glass container and allowed to effor several hours at constant tealiquots of saturated solutions transferred into tared constaine weighed. Solubilities calculate	Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.  (2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that remafter solvent had evaporated.	estimated errors:
	$T/K$ : precision $\pm$ 0.05. $x_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Mahieu, J.	
(2) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	<b></b>	
t/°C x <sub>2</sub> ª	x <sub>1</sub> a	
25.0 0.9893	0.0107	
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 $\pm$ 0.5 (compiler).	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]		Tucker, S.A.; Acree, W.E., Jr.
		Phys. Chem. Liq. <u>1989</u> , 19, 73-79.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	<b>x</b> <sub>2</sub>	$\mathbf{x}_1$
25.0	0.9954	0.00464

# AUXILIARY INFORMATION

## METHOD: APPARATUS/PROCEDURE

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

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

## SOURCE AND PURITY OF MATERIALS:

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

 $x_1$ :  $\pm$  5 % (relative error; compiler).

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

## ESTIMATED ERRORS:

COMPONENTS:		ORIGINAL	Measurements:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]		Smutek, M.; Fris, M.; Fohl, J.			
(2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]		Collection Czech. Chem. Commun. 1967, 32, 931-943.			
VARIABLES:			PREPARED BY:		
T/K = 293, 298, 313 and 333		W.E. Acree, Jr.			
EXPERIMENTAL	VALUES				
t/°C	×2	<b>×</b> 1	t/°C	* <sub>2</sub>	× <sub>1</sub>
20.0	0.9959	0.00411	40.0	0.9916	0.00836
25.0	0.9952	0.00483	60.0	0.9844	0.0156
		AUXILIARY	INFORMATIO	N	<del></del>
METHOD: APPAR	RATUS/PROCEDUR	E	SOURCE AN	D PURITY OF M	ATERIALS:
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from		Czec time to g	h., was recry s from pyridi ive a final p , Commercial	ty, Urxovy Zavady, stallized several ne and cyclohexane writy of 98.3 %. sample, source and od was not specified.	
weight of solid residue that remained after solvent had evaporated.			cision ± 0.05	. rror; compiler).	

COMPONENTS:		ORIGINAL I	ORIGINAL MEASUREMENTS:  Somayajulu, G.R.; Palit, S.R.  J. Phys. Chem. 1954, 58, 417-421.  PREPARED BY:  W.E. Acree, Jr.			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Iodoethane; C <sub>2</sub> H <sub>5</sub> I; [74-88-4] 75-03-6 VARIABLES:						Somayaju
						J. Phys.
						W.E. Acre
EXPERIMENTAL '	VALUES	<del></del>				
T/K	<b>x</b> <sub>2</sub>	* <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	
310.2	0.9881	0.01189	340.2	0.9713	0.02867	
320.2	0.9839	0.01612				
330.2	0.9783	0.02175				
		AUXILI	ARY INFORMATION	N		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AN	D PURITY OF M	MATERIALS:	
Constant tom	Constant temperature bath and a precision			(1) Durity not engelfied 7 m Deless We		

Constant temperature bath and a precision thermometer.

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

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

  (2) Purity not specified, prepared by authors, dried over calcium chloride and distilled before use.

## ESTIMATED ERRORS:

T/K: precision  $\pm$  0.3.  $x_1$ : ± 0.00001 (compiler).

	57		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Acree, W.E., Jr.		
(2) 1-Chlorobutane; C <sub>4</sub> H <sub>9</sub> Cl; [109-69-3]	J. Solution Chem. 1991, 20, 307-318.		
VARIABLES:	PREPARED BY:		
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0 0.9941	0.00586		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) HPLC Grade, 99.5+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.		
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:		

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

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 1,4-Dichlorobutane; C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> ; [110-56-5]		Acree, W.E., Jr.; Zvaigzne, A.I.  Phys. Chem. Liq. 1991, 23, 225-237.		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0	0.9895	0.01053		
METHOD: APPARATUS/PROCEDU		INFORMATION SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.		
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, was stored over molecular sieves and distilled shortly before use.		
Concentrations determine metrically at 356 nm.		ESTIMATED ERRORS:		
		$T/K$ : $\pm$ 0.05. $x_i$ : $\pm$ 1.5 % (relative error).		

08		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.	
<pre>(2) Trichloroethylene; C<sub>2</sub>HCl<sub>3</sub>; [79-01-6]</pre>	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 0.0705		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.	(1) Purity not given, commercial sample of unspecified source, was used as received.	
Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a 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.	
fluorescênce or uv detection.	ESTIMATED ERRORS:	

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

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Iodobenzene; C <sub>6</sub> H <sub>5</sub> I; [591-50-4]		ORIGINAL MEASUREMENTS:  Somayajulu, G.R.; Palit, S.R.  J. Phys. Chem. 1954, 58, 417-421.  PREPARED BY:  W.E. Acree, Jr.						
					/ARIABLES:			
					Temperature			
EXPERIMENTAL	VALUES						•	
T/K	<b>x</b> 2				<b>x</b> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	× <sub>1</sub>
305.2	0.9854	0.01462	320.2	0.9766	0.02344			
310.2	0.9827	0.01728						
315.2	0.9799	0.02014						
		AUXILIARY	INFORMATION	ſ				
METHOD: APPARATUS/PROCEDURE			SOURCE AND	PURITY OF M	IATERIALS:			
Constant temperature bath and a precision thermometer.			(1) Purity not specified, J. T. Baker, USA was recrystallized several times from ethanol and ethyl ethanoate.					
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Reported values computed from variation of mole fraction solubility with temperature.		tallized from toluene. (2) Purity not specified, Columbia Organi Chemicals, was distilled before use.						
		ESTIMATED	ERRORS:					
		T/K: precision ± 0.3. x,: ± 0.00001 (compilier).						

	ວ		
COMPONENTS:	ORIGINAL MEASUREMENTS:  Mahieu, J.  Bull. Soc. Chim. Belgique 1936, 45, 667-677.  PREPARED BY:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]			
(2) Bromobenzene; C <sub>6</sub> H <sub>5</sub> Br; [108-86-1]			
VARIABLES:			
T/K = 298	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
t/°C x <sub>2</sub> ª	x <sub>1</sub> <sup>a</sup>		
25.0 0.9881	0.0119		
a computed by compiler from published so solubilities, which were expressed as w 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 $\pm$ 0.5 (compiler). $x_1$ : $\pm$ 5 % (relative error; compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub>	; [120-12-7]	Mahieu, J.
(2) Chlorobenzene; C <sub>6</sub> H <sub>5</sub> Cl; [108-90-7]		Bull. Soc. Chim. Belgique 1936, 45, 667-677.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
experimental values	$x_2^a$	x <sub>1</sub> ª
25.0	0.9897	0.0103
	ch were expressed	ed solvent compositions and solute as weight percent and grams of
	AUXIL	IARY INFORMATION
METHOD: APPARATUS/PROCEDURE		
METHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:

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

after solvent had evaporated.

(2) Purity and source not given.

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

ESTIMATED ERRORS:

60	
COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</li> <li>Chlorobenzene; C<sub>6</sub>H<sub>5</sub>C1; [108-90-7]</li> </ol>	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 <sup>-3</sup> )
23.0 0.0	628
	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:
	$T/K$ : $\pm$ 1. $c_1$ : $\pm$ 5% (relative error; compiler).

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Methanol; CH <sub>4</sub> O; [67-56-1]		ORIGINAL MEASUREMENTS:		
		Smutek, M.; Fris, M.; Fohl, J.		
		Collection Czech. Chem. Commun. 1967, 32, 931-943.		
VARIABLES:		PREPARED BY:		
T/K = 293		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	<b>*</b> 2	<i>x</i> <sub>1</sub>		
20.0	0.9998	0.000202		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROC	EDURE	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		(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.		

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.

# ESTIMATED ERRORS:

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

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Mahieu, J.
(2) Methanol; CH <sub>4</sub> O; [67-56-1]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C ×2ª	x <sub>1</sub> a
25.0 0.9997	0.000252
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, and a precision balance.	<ol> <li>Purity and source not given.</li> <li>Purity and source not given.</li> </ol>
Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solu-	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Methanol; CH <sub>4</sub> 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	$\sigma_1/(\text{mol dm}^{-3})$
23.0	0.00477
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:

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

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

- 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).

02	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Mahieu, J.
(2) 1-Propanol; C <sub>3</sub> H <sub>8</sub> O; [71-23-8]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°c x <sub>2</sub> ª	ж <sub>1</sub> а
25.0 0.9996	0.000371
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, 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.	(1) Purity and source not given.  (2) Purity and source not given.
	ESTIMATED ERRORS:  T/K: precision ± 0.5 (compiler).  x <sub>1</sub> : ± 5 % (relative error; compiler).

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

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 2-Propanol; C <sub>3</sub> H <sub>8</sub> O; [67-63-0]		Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.
		Fluid Phase Equilibr. <u>1994</u> , 92, 233-253.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>
25.0	0.9996	0.000411
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature k thermometer, and an ul spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 determinetrically at 356 nm.		ESTIMATED ERRORS:
		$T/K: \pm 0.05.$ $x_1: \pm 1.5 \%$ (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Anderson, B.D.
(2) 1-Butanol; C <sub>4</sub> H <sub>10</sub> O; [71-36-3]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
±/°C	(mol dm <sup>-3</sup> )
25.0 0.0	00950
AUXILIAR	( INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.
Excess solute and solvent placed in	(2) puriss, 99.5 %, Fluka Chemical Corpora-
glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	tion, Ronkonkoma, New York, USA, was stored over molecular sieves to remove trace water.

T/K:  $\pm$  0.1 (compiler).  $c_1$ :  $\pm$  3 % (relative error; compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 1-Butanol; C <sub>4</sub> H <sub>10</sub> O; [71-36-3]  VARIABLES:		Zvaigzne, A.I.; Teng, IL.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.  J. Chem. Eng. Data 1993, 38, 389-392.  PREPARED BY:	
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	<b>x</b> <sub>2</sub>	$\mathbf{x_1}$	
25.0	0.9992	0.000801	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.		(2) HPLC Grade, 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use	
Concentrations determi metrically at 356 nm.	ned spectrophoto-	ESTIMATED ERRORS:	
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.  J. Chem. Eng. Data 1994, 39, 114-116.	
(2) 2-Butanol; C <sub>4</sub> H <sub>10</sub> O; [15892-23-6]		
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x <sub>2</sub>	<b>x</b> <sub>1</sub>	
25.0 0.9994	0.000585	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K$ : $\pm 0.05$ . $x_1$ : $\pm 1$ % (relative error).	

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr. (2) 2-Methyl-1-propanol; C<sub>4</sub>H<sub>10</sub>O; [78-83-1] J. Chem. Eng. Data 1994, 39, 541-543. VARIABLES: PREPARED BY: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C **x**<sub>2</sub> x1 0.9995 0.000470 25.0 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath, calorimetric Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. 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. (2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled 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 356 nm. ESTIMATED ERRORS: $T/K: \pm 0.05.$ $x_1$ : $\pm 1.3$ % (relative error).

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

ORIGINAL MEASUREMENTS:

COMPONENTS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Anderson, B.D.
(2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
25.0 0.0	0140
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99.7 %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was used as received.
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.
Concentrations determined spectrophotometrically at 356 nm.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1 (compiler).

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]  VARIABLES:  T/K = 298	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	(mol dm <sup>-3</sup> )
25.0 0.0	118
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:
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).

ORIGINAL MEASUREMENTS:

	6.
COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]  (2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]  VARIABLES:  T/K = 296	ORIGINAL MEASUREMENTS:  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.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
23.0 0.0	117
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 analysi 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) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]		ORIGINAL MEASUREMENTS:	
		Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.  Fluid Phase Equilibr. 1994, 92, 233-253.	
			VARIABLES:
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	<b>x</b> <sub>2</sub>	× <sub>1</sub>	
25.0	0.9978	0.002160	
<del></del>	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDUI	RE .	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.		(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of 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 determined metrically at 356 nm.	spectrophoto-	ESTIMATED ERRORS:	
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).	

- (1) Anthracene; C14H10; [120-12-7]
- (2) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]

### **EVALUATOR:**

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

(USA)

### CRITICAL EVALUATION:

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

### REFERENCES

- Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. Environ. Sci.
- Trechnol. 1990, 24, 639.

  Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay D. Environ. Sci. Technol. 1985, 19, 522.

  Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A. Fluid Phase Equilibr. 1994, 92,
- 233.
- 4. Anderson, B.D., Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, 1978.

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Phenol; C <sub>6</sub> H <sub>6</sub> O; [108-95-2]		ORIGINAL MEASUREMENTS:  Smutek, M.; Fris, M.; Fohl, J.  Collection Czech. Chem. Commun. 1967, 32, 931-943.			
			VARIABLES:		PREPARED BY:
			T/K = 313		W.E. Acree, Jr.
EXPERIMENTAL VALUES					
t/°C	<i>x</i> <sub>2</sub>	× <sub>1</sub>			
40.0	0.9951	0.00487			

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

### SOURCE AND PURITY OF MATERIALS:

- (1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.
- (2) 99 %, Commercial sample, source and purification method was not specified.

### ESTIMATED ERRORS:

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

	69
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.
(2) 1-Hydroxy-2-methylbenzene; C <sub>7</sub> H <sub>8</sub> O; [95-48-7]	Environ. Sci. Technol. 1990, 24, 639-646.
VARIABLES:	PREPARED BY:
T/K = 296	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
23.0 0.0	308
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.

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 2-Propanone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1]		ORIGINAL MEASUREMENTS:	
		Smutek, M.; Fris, M.; Fohl, J.  Collection Czech. Chem. Commun. 1967, 32, 931-943.	
			VARIABLES:
T/K = 293		W.E. Acree, Jr.	
EIPERIMENTAL VALUES			
t/°C	* <sub>2</sub>	× <sub>1</sub>	
20.0	0.9969	0.00313	
20.0	0.9969	0.00313	

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

### SOURCE AND PURITY OF MATERIALS:

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

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

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

### ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> .	: [120-12-7]	Mahieu, J.		
(2) 2-Propanone; C <sub>3</sub> H <sub>8</sub> C	; [67-64-1]	Bull. Soc. Chim. Belgique 1936, 45, 667-677.		
/ARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	<i>x</i> <sub>2</sub> <sup>a</sup>	x <sub>1</sub> a		
		0.00432		
a computed by com	piler from published so ch were expressed as we ams of solvent.			
a computed by compositions, whi	piler from published so ch were expressed as we ams of solvent.	olvent compositions and solute eight percent and grams of		
a computed by composition solubilities, whi solute per 100 gr  METHOD: APPARATUS/PROC Constant temperature and a precision balan	piler from published so the were expressed as we ams of solvent.  AUXILIARY  EDURE  bath, thermometer, ce.  vent placed in closed allowed to equili- rs at constant	olvent compositions and solute eight percent and grams of INFORMATION		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7] (2) 2-Propanone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x <sub>2</sub>	
0.954 0.0	46
AUXILIARY METHOD: APPARATUS/PROCEDURE	INFORMATION SOURCE AND PURITY OF MATERIALS:
No experimental details were given in	(1) Purity and chemical source not speci-
the paper.	fied in paper.
1	
Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	(2) Purity and chemical source not specified in paper.
the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298-	(2) Purity and chemical source not specified in paper.  ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) 2-Butanone; C <sub>4</sub> H <sub>8</sub> O; [78-93-3]	V.V.; Nazarov, V.N.; Vail, E.I.  Sov. Prog. Chem. <u>1986</u> , 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
* <sub>2</sub> * <sub>1</sub>	
0.9953 0.00	247
	J <b>4</b> /
	INFORMATION
AUXILIARY	
AUXILIARY	INFORMATION
AUXILIARY METHOD: APPARATUS/PROCEDURE No experimental details were given in	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298~	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</li> <li>Acetonitrile; C<sub>2</sub>H<sub>3</sub>N; [75-05-8]</li> </ol>	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 <sub>1</sub> /(mol dm <sup>-3</sup> )
23.0	0.00973

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- 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) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Carbon disulfide; CS <sub>2</sub> ; [75-15-0]		Smutek, M.; Fris, M.; Fohl, J.  Collection Czech. Chem. Commun., 1967, 32, 931-943.		
/ARIABLES:		PREPARED BY:		
T/K = 293		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	x <sub>2</sub>	x <sub>1</sub>		
20.0	0.9913	0.00872		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDU	JRE .	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bat and a precision balance Excess solute and solver glass container and allefor several hours at confiquots of saturated stransferred into tared weighed. Solubilities weight of solid residue after solvent had evapor	nt placed in closed owed to equilibrate istant temperature. Dutions were constainers and calculated from that remained	(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.  (2) 99 %, Commercial sample, source and purification method was not specified.  ESTIMATED ERRORS:		
and the state of t		T/K: precision ± 0.05. x,: ± 3 % (relative error; compiler).		

COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Anthrace	ne; C <sub>14</sub> H <sub>10</sub> ; [1	20-12-7]	Doane, E.P.; Drickamer, H.G.		
(2) Carbon disulfide; CS <sub>2</sub> ; [75-15-0]		J. Phys. Chem. <u>1955</u> , 59, 454-457.			
VARIABLES:			PREPARED E	BY:	
T/K = 298, P	ressure		W.E. Acree, Jr.		
EXPERIMENTAL '	VALUES				
P/atm	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	P/atm	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>
1	0.9916	0.0084	2000	0.9973	0.0027
240	0.9930	0.0070	4000	0.9987	0.0013
500	0.9941	0.0059			
1000	0.9959	0.0041			
		AUXILIARY	INFORMATION	4	
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF N	MATERIALS:
balance and	Constant temperature bath, analytical balance and high pressure equipment.		Compa	st grade, Eas any, Rocheste as received.	stman 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,		(2) C.P. grade, J.T. Baker, was dried over phosphorous pentoxide and distilled.			
solvent evap	orated to dry	ness, and con- eight of solid	$x_1: \pm 1-3$	cision ± 0.1.	heric pressure, and the pressures.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,	
(2) Acetic anhydride; C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> ;	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44.	
[108-24-7]	(English Translation)	
/ARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$x_2$ $x_1$		
0.9972 0.00	128	
5.5.12	720	
	INFORMATION	
AUXILIARY		
AUXILIARY	INFORMATION	
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7] (2) Dimethylsulfoxide; C <sub>2</sub> H <sub>6</sub> OS; [67-68-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$\mathbf{x}_2 \mathbf{x}_1$	
0.9979 0.00	021
	INFORMATION SOURCE AND PURITY OF MATERIALS.
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</li> <li>(2) Dimethyl sulfoxide; C<sub>2</sub>H<sub>6</sub>SO; [67-68-5]</li> </ul>	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 <sup>-3</sup> )
23.0 0.0	315
AUXILIARY	INFORMATION
METROD: 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.
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-	

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Mahieu, J.
(2) Nitrobenzene; C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> ; [98-95-3]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub> a	*1ª
25.0 0.9897	0.01032
2010	***************************************
a computed by compiler from put solubilities, which were expres solute per 100 grams of solvent	lished solvent compositions and solute
a computed by compiler from put solubilities, which were expres solute per 100 grams of solvent	lished solvent compositions and solute seed as weight percent and grams of
a computed by compiler from put solubilities, which were expres solute per 100 grams of solvent	lished solvent compositions and solute used as weight percent and grams of  AUXILIARY INFORMATION  SOURCE AND PURITY OF MATERIALS: eter, (1) Purity and source not given.
a computed by compiler from put solubilities, which were expressionable per 100 grams of solvent solute per 100 grams of solvent METHOD: APPARATUS/PROCEDURE  Constant temperature bath, thermome and a precision balance.  Excess solute and solvent placed in glass containers and allowed to equipate for several hours at constant temperature. Aliquots of saturature	clished solvent compositions and solute seed as weight percent and grams of  AUXILIARY INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and source not given.  (2) Purity and source not given.
a computed by compiler from put solubilities, which were expressionally solute per 100 grams of solvent METHOD: APPARATUS/PROCEDURE  Constant temperature bath, thermomerand a precision balance.  Excess solute and solvent placed in glass containers and allowed to embrate for several hours at constant	lished solvent compositions and solute used as weight percent and grams of  AUXILIARY INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and source not given.  (2) Purity and source not given.  (2) Purity and source not given.  (3) Purity and source not given.  (4) Estimated from ESTIMATED ERRORS:

ORIGINAL MEASUREMENTS:

### ORIGINAL MEASUREMENTS: COMPONENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H. (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] (2) Nitrobenzene; C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>; [98-95-3] Environ. Sci. Technol. 1990, 24, 639-646. VARIABLES: PREPARED BY: T/K = 296W.E. Acree, Jr. EXPERIMENTAL VALUES $c_1/(\text{mol dm}^{-3})$ t/°C 0.0738 23.0 AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection. Purity not given, commercial sample of unspecified source, was used as received. Excess solute and solvent were placed in glass vials and allowed to equilibrate (2) Purity and chemical source not given, purification procedure not specified. with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or my detection fluorescence or uv detection. ESTIMATED ERRORS: T/K: ± 1.

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

ORIGINAL MEASUREMENTS:

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Anthraces	ne; C <sub>14</sub> H <sub>10</sub> ; [1	20-12-7]	Srivastava, R.D.; Gupta, P.D.			
(2) Nitrobenzene; C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> ; [98-95-3]		J. Indian Chem. Soc. <u>1967</u> , 44, 960-963.				
ARIABLES:		PREPARED BY:				
Temperature	Temperature		W.E. Acree, Jr.			
EXPERIMENTAL V	/ALUES					
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sup>5</sup>	<i>*</i> 1	
286.2	0.9931	0.00688	307.4	0.9846	0.01545	
289.8	0.9908	0.00916	308.2	0.9839	0.01614	
296.2	0.9890	0.01104	313.0	0.9811	0.01892	
298.2	0.9885	0.01152				
	<del></del>	AUXILIARY	INFORMATION	ľ		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath and a precision thermometer.		<ol> <li>Purity not given, British Drug Houses, United Kingdom, was recrystallized and sublimed.</li> <li>Purity not given, British Drug Houses, was dried and distilled.</li> </ol>				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by						
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
craca or sort	ra sorare are	appeared.		ision <u>+</u> 0.1. (relative e	rror, Compiler).	

COMPONENTS:

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene	; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Mahieu, J.
(2) Aniline; C	<sub>3</sub> H <sub>7</sub> N; [62-53-3]	Bull. Soc. Chim. Belgique <u>1936</u> , 45, 667-677.
VARIABLES:		PREPARED BY:
T/K = 298 and 3	313	W.E. Acree, Jr.
EXPERIMENTAL VA	LUES	
t/°C	$x_2^a$	$x_1^a$
25.0	0.9961	0.00390
40.0	0.9923	0.00773
a computed	by compiler from publ	ished solvent compositions and solute
solubilitie	es, which were express 100 grams of solvent.	ished solvent compositions and solute ed as weight percent and grams of .  XILLIARY INFORMATION
solubilitie	es, which were express 100 grams of solvent.	ed as weight percent and grams of
solubilities solute per  METHOD: APPARAT  Constant tempe and a precision  Excess solute glass containe brate for seve	AU  US/PROCEDURE  rature bath, thermomet	SOURCE AND PURITY OF MATERIALS:  (1) Purity and source not given.  (2) Purity and source not given.

COMPONENTS:		ORIGINAL MEASUREMENTS:								
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]  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		<u> </u>		
					T/K	<b>*</b> 2	× <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>
313.5	0.9833	0.0167	353.1	0.9470	0.0530					
326.7	0.9758	0.0242	359.0	0.9415	0.0585					
337.4	0.9674	0.0326								
344.5	0.9603	0.0397								
		AUXILIARY	INFORMATION	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		Milwa talli (2) Gold Compa	ukee, Wiscon ized from tol Label, 99.9+ any, was used	Chemical Company, sin, USA, was recrysuene.  *, Aldrich Chemical as received.						
noting the to	emperature at id solute dis	which the last appeared.	T/K: prec x <sub>1</sub> : ± 0.0	cision + 0.1.						

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]  VARIABLES:		Smutek, M.; Fris, M.; Fohl, J.		
		Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.		
		PREPARED BY:		
T/K = 293 and 333		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	x <sub>2</sub>	<i>x</i> <sub>1</sub>		
20.0	0.9917	0.00834		
60.0	0.9716	0.0284		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	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) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.  (2) 99 %, Commercial sample, source and purification method was not specified.		
weight of solid residu after solvent had evan	e that remained	ESTIMATED ERRORS:		
		$T/K$ : precision $\pm$ 0.05. $x_1$ : $\pm$ 3 % (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<ul> <li>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-17-7]</li> <li>(2) Pyridine; C<sub>5</sub>H<sub>5</sub>N; [110-86-1]</li> </ul>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)		
VARIABLES:	PREPARED BY:		
T/K = See below	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
x <sub>2</sub>			
0.989 0.0	11		
AUXILIARY	INFORMATION		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-		
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-		

8			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>12</sub> H <sub>10</sub> ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.  Sov. Prog. Chem. 1986, 52, 41-44.		
17 10			
(2) Quinoline; C <sub>9</sub> H <sub>7</sub> N; [91-22-5]	(English Translation)		
ARIABLES:	PREPARED BY:		
T/K = See below	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
$x_2$ $x_1$			
0.989 0.0	11		
AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.		
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.		
	ESTIMATED ERRORS:		
	T/K: Unknown. x,: ± 8 % (relative error; compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]  VARIABLES: Temperature		McLaughli	n, E.	W.B.; Auwaerter, J.E.; 88, 16, 519-534.	
		PREPARED BY: W.E. Acree, Jr.			
					EXPERIMENTAL V
T/K	<i>x</i> <sub>2</sub>	* <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>
297.4	0.9895	0.0105	351.8	0.9506	0.0494
317.9	0.9798	0.0202	358.1	0.9430	0.0570
332.9	0.9697	0.0303			
337.0	0.9659	0.0341			
		AUXILIARY	INFORMATION	ſ	
METHOD: APPARATUS/PROCEDURE  Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		(1) 99.99 Milwa talli (2) Gold Compa	Label, 99.9+ any, was used  ERRORS:	Chemical Company, sin, USA, was recrystuene.  %, Aldrich Chemical as received.	

(1) Anthracene; $C_{14}H_{10}$ ; [120-17-7] (2) Methoxybenzene; $C_7H_8O$ ; [100-66-3]  VARIABLES: $T/K$ = See below	ORIGINAL MEASUREMENTS:  Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.  Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)  PREPARED BY: W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub>		
0.9898 0.0	102	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-17-7]</li> <li>1-Methyl-2-pyrrolidinone; C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]</li> </ol>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$x_2$ $x_1$	
0.975 0.03	25
	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
	(2) Purity and chemical source not speci-
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	fied in paper.
the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298-	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>12</sub> H <sub>10</sub> ; [120-17-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,		
14 10	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44.		
(2) N,N-Dimethylacetamide; C <sub>4</sub> H <sub>9</sub> NO; [127-19-5]	(English Translation)		
/ARIABLES:	PREPARED BY:		
T/K = See below	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
$x_2$ $x_1$			
0.986 0.03	1.4		
	INFORMATION		
AUXILIARY	INFORMATION		
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-		
AUXILIARY  METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-		

	ORIGINAL MEASUREMENTS:		
<ul> <li>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-17-7]</li> <li>(2) N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]</li> </ul>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)		
VARIABLES:	PREPARED BY:		
T/K = See below	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
$x_2$ $x_1$			
0.991 0.00	99		
AUXILIARY	INFORMATION		
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-		
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:		
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-		

	0
COMPONENTS:  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7]  (2) Tetramethylene sulfone; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S; [126-33-0]  VARIABLES:  T/K = See below	ORIGINAL MEASUREMENTS:  Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)  PREPARED BY:  W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$x_2$ $x_1$	
0.9964 0.0	036
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-17-7] (2) Tributyl phosphate; C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P; [126-73-8]  VARIABLES:  T/K = See below	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.  Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)  PREPARED BY:  W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x <sub>2</sub>	
0.989 0.0	11
AUXILIARY METHOD: APPARATUS/PROCEDURE	INFORMATION SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).

ORIGINAL MEASUREMENTS:

(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) 1,2,3,5-Tetranitrobenzene; C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>8</sub> ; [3698-53-1]		ORIGINAL MEASUREMENTS:		
		Shinomiya, C.		
		J. Chem. Soc. Japan 1940, 15, 259-270.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>		
399.2	1.000	0.000		
398.2	0.935	0.065		
418.2	0.842	0.158		
436.2	0.693	0.307		
442.2	0.604	0.396		
444.2	0.487	0.513		
441.7	0.430	0.570		
449.2	0.354	0.646		
459.2	0.301	0.699		
462.2	0.271	0.729		
490.2	0.000	1.000		

Author reports formation of a 1:1 anthracene - 1,2,3,5-tetranitrobenzene molecular compound having a melting point temperature of 444.2 K. Two eutectic points occur at  $x_1$  = 0.055 and T/K = 393.7, and at  $x_1$  = 0.605 and T/K = 436.2.

# AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE No experimental details given in paper. (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<sub>1</sub>: ± 0.002 (Compiler).

ORIGINAL MEASUREMENTS:
Singh, N.P.; Shukla, B.M.
Cryst. Res. Technol. <u>1985</u> , 20, 345-349.
PREPARED BY:
W.E. Acree, Jr.

### EXPERIMENTAL VALUES

Phase equilibrium data not given in cited paper. Authors report formation of a 1:1 anthracene - 2,4,6-trinitrophenol molecular compound having a melting point temperature of 413.2 K. Two eutectic points occur at  $x_1 = 0.1017$  and T/K = 382.7, and at  $x_1 = 0.6250$  and T/K = 403.2.

AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Binary mixtures were prepared by weight. Melting and thaw point temperatures determined by the method of Rastogi et	(1) Purity and chemical source not specified in paper.
al. (see J. Cryst. Growth <u>1977</u> , 40, 329).	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	$T/K$ : precision $\pm$ 0.3 (Compiler). $x_1$ : $\pm$ 0.0002 (Compiler).

- (1) Anthracene; C1/H10; [120-12-7]
- (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1]
- (3) 2,2,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]

### ORIGINAL MEASUREMENTS:

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

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

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

t = 25.0 °C

,	(s)	x <sub>3</sub>	<i>x</i> <sub>1</sub>
	0.0000	0.0000	0.001978
(	0.1093	0.1091	0.001899
(	0.2115	0.2111	0.001809
(	0.3862	0.3856	0.001651
(	0.5049	0.5041	0.001536
(	0.6142	0.6133	0.001429
	0.8099	0.8089	0.001249
	0.8961	0.8951	0.001163
	1.0000	0.9989	0.001074

 $<sup>^</sup>a$   $x_3^{\,(s)};$  initial mole fraction of binary solvent mixture;  $x_1;$  mole fraction solubility of the solute;  $x_3;$  mole fraction of component 3 in the ternary solution.

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) HPLC Grade, 99.7 %, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_3^{(s)}$ :  $\pm$  0.0001.  $x_1$ :  $\pm$  1 % (relative error).

- (1) Anthracene; C14H10; [120-12-7]
- (2) n-Hexane;  $C_6H_{14}$ ; [110-54-3]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C

x <sub>3</sub> <sup>(s)</sup>	<i>x</i> <sub>3</sub>	x <sub>1</sub>
0.0000	0.0000	0.001274
0.1751	0.1749	0.001288
0.3162	0.3158	0.001237
0.5447	0.5441	0.001071
0.6331	0.6325	0.000990
0.7297	0.7290	0.000898
0.8712	0.8706	0.000740
0.9411	0.9435	0.000661
1.0000	0.9994	0.000591

 $<sup>^</sup>a$   $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_3^{(s)}$ :  $\pm$  0.0001.  $x_1$ :  $\pm$  1 % (relative error).

- (1) Anthracene; C14H10; [120-12-7]
- (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5] (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	x <sub>1</sub>
0.0000	0.0000	0.001571
0.1719	0.1716	0.001566
0.3272	0.3267	0.001456
0.5674	0.5667	0.001182
0.6622	0.6615	0.001077
0.7444	0.7437	0.000953
0.8824	0.8817	0.000762
0.9398	0.9392	0.000681
1.0000	0.9994	0.000591

 $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_4$ : 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 equili-brium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophoto-metrically at 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 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:

 $T/K: \pm 0.05.$  $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1 \%$  (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
- (3) 1-Propanol; C<sub>3</sub>H<sub>3</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

### t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> 3	<b>*</b> 1
0.0000	0.0000	0.001838
0.1908	0.1905	0.001779
0.3483	0.3477	0.001632
0.5892	0.5884	0.001300
0.6806	0.6798	0.001145
0.7661	0.7653	0.001013
0.8939	0.8932	0.000784
0.9477	0.9471	0.000682
1.0000	0.9994	0.000591

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

 $T/K: \pm 0.05.$   $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1 \%$  (relative error).

### 88 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] J. Chem. Eng. Data 1993, 38, 389-392. (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES<sup>a</sup> $t = 25.0 \, {}^{\circ}\text{C}$ x,(s) $x_3$ $x_1$ 0.0000 0.0000 0.001553 0.1335 0.1333 0.001576

0.001543

0.001288

0.001150

0.001010

0.000795

0.000699

0.000591

<sup>a</sup>  $x_3^{(s)}$ : 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

0.2567

0.4886

0.5890

0.6893

0.8511

0.9226

1.0000

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

0.2563

0.4880

0.5883

0.6886

0.8504

0.9220

0.9994

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

 $T/K: \pm 0.05.$  $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1 % (relative error).$ 

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>; [108-87-2]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

•	_	25	^	00
C	=	23	. U	

x <sub>3</sub> (s)	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001649
0.1539	0.1536	0.001697
0.2943	0.2938	0.001578
0.5326	0.5319	0.001294
0.6305	0.6298	0.001154
0.7206	0.7199	0.001018
0.8687	0.8680	0.000781
0.9328	0.9322	0.000687
1.0000	0.9994	0.000591

a  $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

T/K:  $\pm 0.05$ .  $x_3^{(s)}$ :  $\pm 0.0001$ .  $x_1$ :  $\pm 1$  % (relative error).

### 90 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C, H, 10; [120-12-7] Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. (2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; J. Chem. Eng. Data 1993, 38, 389-392. [540-84-1] (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C x3<sup>(s)</sup> $x_3$ $\mathbf{x}_1$ 0.0000 0.0000 0.001074 0.2141 0.2139 0.001089 0.3510 0.3506 0.001057 0.5891 0.5886 0.000929 0.6884 0.6878 0.000862 0.7911 0.7905 0.000783 0.8968 0.8962 0.000693 0.9454 0.9448 0.000649 1.0000 0.9994 0.000591 $^a$ $x_3^{(s)}$ : initial mole fraction of binary solvent mixture; $x_1$ : mole fraction solubility of the solute; $x_3$ : mole fraction of component 3 in the ternary solution. **AUXILIARY INFORMATION**

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_3^{(s)}$ :  $\pm$  0.0001.  $x_1$ :  $\pm$  1 % (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

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

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

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

t = 25.0	°C
----------	----

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001978
0.2089	0.2085	0.001958
0.3695	0.3688	0.001792
0.6061	0.6052	0.001423
0.7002	0.6993	0.001250
0.7780	0.7771	0.001100
0.9021	0.9014	0.000824
0.9537	0.9530	0.000706
1.0000	0.9994	0.000591

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

 $T/K: \pm 0.05.$   $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1$  % (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>*</i> 1
0.0000	0.0000	0.001274
0.1739	0.1737	0.001271
0.3076	0.3072	0.001201
0.5342	0.5337	0.000987
0.6314	0.6308	0.000873
0.7185	0.7179	0.000767
0.8700	0.8695	0.000581
0.9391	0.9386	0.000490
1.0000	0.9996	0.000411

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

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

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

			_	_
+	=	25	. ດ	O.C.

x <sub>3</sub> <sup>(8)</sup>	<i>x</i> <sub>3</sub>	$x_1$
0.0000	0.0000	0.001571
0.1851	0.1848	0.001499
0.3256	0.3252	0.001371
0.5575	0.5569	0.001102
0.6607	0.6601	0.000956
0.7381	0.7375	0.000836
0.8861	0.8856	0.000603
0.9416	0.9411	0.000509
1.0000	0.9996	0.000411
	0.1851 0.3256 0.5575 0.6607 0.7381 0.8861 0.9416	0.0000       0.0000         0.1851       0.1848         0.3256       0.3252         0.5575       0.5569         0.6607       0.6601         0.7381       0.7375         0.8861       0.8856         0.9416       0.9411

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

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

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

t = 25.0 °C

x3(e)	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001838
0.2157	0.2153	0.001690
0.3580	0.3574	0.001540
0.5840	0.5833	0.001206
0.6874	0.6867	0.001025
0.7670	0.7663	0.000868
0.8928	0.8922	0.000622
0.9478	0.9473	0.000515
1.0000	0.9996	0.000411

 $<sup>^</sup>a$   $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

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

## COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, (2) Cyclohexane; C<sub>4</sub>H<sub>12</sub>; [110-82-7] Fluid Phase Equilibr. 1994, 92, 233-253. (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES t = 25.0 °C 3

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<b>×</b> 1
0.0000	0.0000	0.001553
0.1430	0.1428	0.001568
0.2666	0.2662	0.001474
0.4882	0.4876	0.001213
0.5897	0.5891	0.001051
0.6817	0.6811	0.000899
0.8463	0.8458	0.000639
0.9239	0.9234	0.000519
1.0000	0.9996	0.000411

 $<sup>^{</sup>a}$   $x_{3}^{(s)}$ : 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 temperature. 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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Methylcyclohexane; C <sub>7</sub> H <sub>14</sub> ; [108-87-2] (3) 2-Propanol; C <sub>3</sub> H <sub>8</sub> O; [67-63-0]		Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker S.A.  Fluid Phase Equilibr. 1994, 92, 233-253		
VARIABLES:	-	PREPARED BY:		
T/K = 298, Solvent composition		W.E. Acree, Jr.		
EXPERIMENTAL VALU  t = 25.0 °C				
x <sub>3</sub> (s)	*3	×1 .		
0.0000	0.0000	0.001649		
0.1518	0.1515	0.001683		
0.2965	0.2960	0.001536		
0.5234	0.5228	0.001226		
0.6234	0.6227	0.001055		
0.7170	0.7164	0.000887		
0.8649	0.8644	0.000631		
0.9375	0.9370	0.000508		

# a $x_3^{(s)}$ : initial mole fraction of binary solvent mixture; $x_1$ : mole fraction solubility of the solute; $x_3$ : mole fraction of component 3 in the ternary solution.

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

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

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

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

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 2,2,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES

t	=	25.	0	°C

x3 <sup>(s)</sup>	x <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001074
0.1997	0.1995	0.001054
0.3535	0.3532	0.000988
0.5865	0.5860	0.000839
0.6809	0.6804	0.000751
0.7676	0.7671	0.000664
0.8932	0.8927	0.000535
0.9492	0.9488	0.000471
1.0000	0.9996	0.000411

 $<sup>^{</sup>a}$   $x_{3}^{\,(s)}\colon$  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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

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

- (1) Anthracene; C14H10; [120-12-7]
- (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

### ORIGINAL MEASUREMENTS:

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

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

### VARIABLES:

T/K = 298, Solvent composition

### PREPARED BY:

W.E. Acree, Jr.

### EXPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C

x3 <sup>(s)</sup>	x <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001978
0.2154	0.2150	0.001978
0.3666	0.3660	0.001760
0.5948	0.5940	0.001335
0.6912	0.6904	0.001152
0.7744	0.7737	0.000948
0.8963	0.8957	0.000660
0.9537	0.9532	0.000526
1.0000	0.9996	0.000411

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

### ESTIMATED ERRORS:

 $x_3^{(s)}$ :  $\pm 0.05$ .  $x_3^{(s)}$ :  $\pm 0.0001$ .  $x_1$ :  $\pm 1$  % (relative error).

- (1) Anthracene; C14H10; [120-12-7]
- (2) n-Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]
- (3) 1-Butanol; C<sub>4</sub>H<sub>10</sub>O; [71-36-3]

#### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

x3 <sup>(s)</sup>	x <sub>3</sub>	×1
0.0000	0.0000	0.001274
0.1460	0.1458	0.001316
0.2668	0.2665	0.001310
0.4876	0.4870	0.001218
0.5800	0.5793	0.001162
0.6804	0.6797	0.001068
0.8479	0.8471	0.000931
0.9247	0.9239	0.000857
1.0000	0.9992	0.000801

 $<sup>^{</sup>a}$   $x_{3}^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_{1}$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### **ESTIMATED ERRORS:**

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5]
- (3) 1-Butanol; C4H10O; [71-36-3]

#### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

#### t = 25.0 °C

(s)		
*3 <sup>(s)</sup>	x <sup>3</sup>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001571
0.1562	0.1560	0.001576
0.2876	0.2872	0.001511
0.5171	0.5164	0.001333
0.6174	0.6166	0.001230
0.7033	0.7025	0.001142
0.8622	0.8614	0.000972
0.9315	0.9307	0.000886
1.0000	0.9992	0.000801

 $<sup>^</sup>a$   $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
- (3) 1-Butanol; C<sub>4</sub>H<sub>10</sub>O; [71-36-3]

#### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(8)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001838
0.1645	0.1642	0.001828
0.3070	0.3065	0.001725
0.5368	0.5360	0.001467
0.6389	0.6380	0.001336
0.7313	0.7304	0.001207
0.8738	0.8729	0.000998
0.9365	0.9357	0.000892
1.0000	0.9992	0.000801

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (3) 1-Butanol; C<sub>4</sub>H<sub>10</sub>O; [71-36-3]

#### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES®

t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001553
0.1151	0.1149	0.001622
0.2108	0.2105	0.001586
0.4380	0.4374	0.001414
0.5390	0.5383	0.001291
0.6811	0.6803	0.001152
0.8255	0.8247	0.000978
0.9086	0.9078	0.000895
1.0000	0.9992	0.000801
	0.1151 0.2108 0.4380 0.5390 0.6811 0.8255	0.0000       0.0000         0.1151       0.1149         0.2108       0.2105         0.4380       0.4374         0.5390       0.5383         0.6811       0.6803         0.8255       0.8247         0.9086       0.9078

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>; [108-87-2]
- (3) 1-Butanol; C<sub>4</sub>H<sub>10</sub>O; [71-36-3]

#### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree. Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

t	=	25.	0	°C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	x <sub>1</sub>
0.0000	0.0000	0.001649
0.1358	0.1356	0.001710
0.2675	0.2671	0.001671
0.4783	0.4776	0.001453
0.5740	0.5732	0.001329
0.6764	0.6756	0.001193
0.8449	0.8441	0.000995
0.9221	0.9213	0.000892
1.0000	0.9992	0.000801

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 2,2,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]
- (3) 1-Butanol; C<sub>4</sub>H<sub>10</sub>O; [71-36-3]

#### ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, 38, 389-392.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001074
0.1567	0.1565	0.001125
0.3031	0.3028	0.001121
0.5376	0.5370	0.001051
0.6387	0.6381	0.000996
0.7330	0.7323	0.000956
0.8819	0.8811	0.000870
0.9443	0.9435	0.000838
1.0000	0.9992	0.000801

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

#### ORIGINAL MEASUREMENTS: COMPONENTS: Zvaigzne, A.I.; Acree, W.E., Jr. (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1] J. Chem. Eng. Data 1994, 39, 117-118. (3) 1-Butanol; C4H10O; [71-36-3] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES t = 25.0 °C x3<sup>(s)</sup> x, $x_3$ 0.0000 0.001978 0.0000 0.001977 0.1882 0.1878 0.001855 0.3325 0.3319 0.5540 0.5531 0.001561 0.6547 0.6538 0.001405

 $^a$   $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_5$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

0.001265

0.001010

0.000918

0.000801

#### METHOD: APPARATUS/PROCEDURE

0.7426

0.8842

0.9413

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

0.7417

0.8833

0.9404

0.9992

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

 $x_3^{(s)}$ :  $\pm 0.05$ .  $x_3^{(s)}$ :  $\pm 0.0001$ .  $x_1$ :  $\pm 1$  % (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 114-116.

#### **VARIABLES:**

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001274
0.1432	0.1430	0.001311
0.2657	0.2654	0.001282
0.4851	0.4845	0.001169
0.5863	0.5857	0.001070
0.6820	0.6813	0.000969
0.8497	0.8490	0.000770
0.9249	0.9243	0.000676
1.0000	0.9994	0.000585

 $<sup>^</sup>a$   $x_3^{\,(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Heptane; C7H16; [142-82-5]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 114-116.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t =	25.0	°C
-----	------	----

*3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	× <sub>1</sub>
0.0000	0.0000	0.001571
0.1599	0.1597	0.001541
0.2887	0.2883	0.001476
0.5182	0.5175	0.001280
0.6157	0.6150	0.001163
0.7059	0.7052	0.001041
0.8693	0.8686	0.000784
0.9328	0.9322	0.000685
1.0000	0.9994	0.000585

 $<sup>^</sup>a$   $x_3^{(s)};$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 114-116.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	*3	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001838
0.1724	0.1721	0.001783
0.3201	0.3196	0.001658
0.5408	0.5400	0.001412
0.6384	0.6376	0.001263
0.7265	0.7257	0.001111
0.8791	0.8784	0.000826
0.9353	0.9346	0.000717
1.0000	0.9994	0.000585

 $<sup>^</sup>a$   $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 114-116.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUESa

t = 25.0 °C

*3 <sup>(s)</sup>	*3	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001553
0.1266	0.1264	0.001618
0.2285	0.2281	0.001565
0.4422	0.4416	0.001370
0.5429	0.5422	0.001247
0.6425	0.6418	0.001088
0.8210	0.8203	0.000829
0.9089	0.9083	0.000699
1.0000	0.9994	0.000585

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

#### 110 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C14H10; [120-12-7] Zvaigzne, A.I.; Acree, W.E., Jr. (2) Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>; [108-87-2] J. Chem. Eng. Data 1994, 39, 114-116. (3) 2-Butanol; C,H100; [15892-23-6] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C x,(s) $x_3$ X1 0.0000 0.0000 0.001649 0.1460 0.1457 0.001725

0.2585 0.2581 0.001647 0.4740 0.4733 0.001413 0.5832 0.5825 0.001262 0.6743 0.6735 0.001117 0.8541 0.8534 0.000821 0.9234 0.9227 0.000705

0.9994

#### AUXILIARY INFORMATION

0.000585

#### METHOD: APPARATUS/PROCEDURE

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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

 $<sup>^</sup>a$   $x_3^{(s)}$ : 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.

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 2,2,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 114-116.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<i>×</i> 1
0.0000	0.0000	0.001074
0.1574	0.1572	0.001116
0.3118	0.3115	0.001091
0.5396	0.5391	0.001000
0.6365	0.6359	0.000935
0.7292	0.7286	0.000863
0.8766	0.8760	0.000720
0.9475	0.9469	0.000646
1,0000	0.9994	0.000585

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

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

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<i>*</i> 1
0.0000	0.0000	0.001978
0.1795	0.1791	0.001977
0.3264	0.3258	0.001833
0.5520	0.5512	0.001513
0.6528	0.6519	0.001343
0.7394	0.7385	0.001167
0.8794	0.8786	0.000854
0.9348	0.9341	0.000735
1.0000	0.9994	0.000585

 $<sup>^{8}</sup>$   $x_{3}^{(s)};$  initial mole fraction of binary solvent mixture;  $x_{1};$  mole fraction solubility of the solute;  $x_{3};$  mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) n-Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]
- (3) 2-Methyl-1-propanol; C<sub>4</sub>H<sub>10</sub>O; [78-83-1]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 541-543.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

x <sub>3</sub> (s)	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001274
0.1473	0.1471	0.001299
0.2688	0.2685	0.001236
0.4807	0.4802	0.001063
0.5889	0.5883	0.000947
0.6846	0.6840	0.000838
0.8524	0.8519	0.000645
0.9250	0.9245	0.000560
1.0000	0.9995	0.000470

 $<sup>^</sup>a$   $x_3^{(s)}$ ; initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### **AUXILIARY INFORMATION**

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C14H10; [120-12-7] Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr. (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5] J. Chem. Eng. Data 1994, 39, 541-543. (3) 2-Methyl-1-propanol; C,H100; [78-83-1] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUESa t = 25.0 °C

x <sub>3</sub> (s)	<i>x</i> <sub>3</sub>	<b>x</b> 1
0.0000	0.0000	0.001571
0.1644	0.1642	0.001514
0.2825	0.2821	0.001435
0.5123	0.5117	0.001181
0.6094	0.6088	0.001031
0.7105	0.7099	0.000899
0.8567	0.8561	0.000680
0.9294	0.9289	0.000575
1.0000	0.9995	0.000470

 $<sup>^{8}</sup>$   $x_{3}^{(s)}$ : 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 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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C14H10; [120-12-7] Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr. (2) n-Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9] J. Chem. Eng. Data 1994, 39, 541-543. (3) 2-Methyl-1-propanol; C<sub>L</sub>H<sub>10</sub>O; [78-83-1] PREPARED BY: VARIABLES: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001838
0.1786	0.1783	0.001742
0.3077	0.3072	0.001601
0.5373	0.5366	0.001278
0.6371	0.6364	0.001111
0.7281	0.7274	0.000955
0.8741	0.8735	0.000693
0.9385	0.9380	0.000581
1.0000	0.9995	0.000470

 $<sup>^</sup>a$   $x_3^{(s)}$ : 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 spectrophoto-metrically at 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, 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:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr
(2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]	J. Chem. Eng. Data 1994, 39, 541-543.
(3) 2-Methyl-1-propanol; C <sub>4</sub> H <sub>10</sub> O; [78-83-1]	J. Chem. Big. Data <u>1994</u> , 39, 541-343.
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.

x <sub>3</sub> <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001553
0.1267	0.1265	0.001565
0.2262	0.2259	0.001488
0.4297	0.4292	0.001232
0.5441	0.5435	0.001073
0.6400	0.6394	0.000928
0.8155	0.8149	0.000692
0.9131	0.9126	0.000575
1.0000	0.9995	0.000470

a  $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>; [108-87-2]
- (3) 2-Methyl-1-propanol; C<sub>4</sub>H<sub>10</sub>O; [78-83-1]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 541-543.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EIPERIMENTAL VALUES

t	=	25	.0	°C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<b>*</b> 1
0.0000	0.0000	0.001649
0.1438	0.1436	0.001697
0.2568	0.2564	0.001568
0.4769	0.4763	0.001265
0.5837	0.5831	0.001100
0.6739	0.6733	0.000963
0.8428	0.8422	0.000693
0.9143	0.9138	0.000590
1.0000	0.9995	0.000470

 $<sup>^{8}</sup>$   $x_{3}^{(8)}$ : initial mole fraction of binary solvent mixture;  $x_{1}$ : mole fraction solubility of the solute;  $x_{3}$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

#### 118 ORIGINAL MEASUREMENTS: COMPONENTS: Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr. (1) Anthracene; C14H10; [120-12-7] (2) 2,2,4-Trimethylpentane; C8H18; J. Chem. Eng. Data 1994, 39, 541-543. [540-84-1] (3) 2-Methyl-1-propanol; C4H10O; [78-83-1] PREPARED BY: VARIABLES: W.E. Acree, Jr. T/K = 298, Solvent composition EXPERIMENTAL VALUES t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001074
0.1859	0.1857	0.001087
0.3227	0.3224	0.001019
0.5402	0.5397	0.000880
0.6451	0.6446	0.000805
0.7334	0.7329	0.000730
0.8780	0.8775	0.000591
0.9413	0.9408	0.000536
1.0000	0.9995	0.000470

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1]
- (3) 2-Methyl-1-propanol; C<sub>4</sub>H<sub>10</sub>O; [78-83-1]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1994, 39, 541-543.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(8)</sup>	<b>x</b> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001978
0.1860	0.1856	0.001892
0.3238	0.3232	0.001716
0.5548	0.5541	0.001336
0.6531	0.6523	0.001150
0.7351	0.7344	0.000990
0.8806	0.8800	0.000699
0.9449	0.9444	0.000574
1.0000	0.9995	0.000470

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

14

#### COMPONENTS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Hexane; C<sub>A</sub>H<sub>1</sub>, [110-54-3]
- (3) 3-Methyl-1-butanol; C<sub>5</sub>H<sub>12</sub>O; [123-51-3]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data, in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001274
0.1275	0.1273	0.001341
0.2355	0.2352	0.001312
0.4384	0.4379	0.001221
0.5447	0.5441	0.001146
0.6401	0.6394	0.001064
0.8269	0.8262	0.000890
0.9115	0.9108	0.000813
1.0000	0.9993	0.000727

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene; C14	H <sub>10</sub> ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5] (3) 3-Methyl-1-butanol; C <sub>5</sub> H <sub>12</sub> O; [123-51-3]		J. Chem. Eng. Data, in press.
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALUES <sup>8</sup> t = 25.0 °C	ı	
*3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	x <sub>1</sub>
0.0000	0.0000	0.001571
0.1431	0.1429	0.001554
0.2545	0.2541	0.001500
0.4751	0.4745	0.001337
0.5713	0.5706	0.001234
0.6681	0.6674	0.001128
0.8383	0.8375	0.000916
	0.9143	0.000823
0.9151		

# $^a$ $x_3^{\,(s)}\colon$ 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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

122		
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Anthracene;	C <sub>14</sub> H <sub>10</sub> ; [120-12-7]	Zvaigzne, A.I.; Acree, W.E., Jr.
(2) n-Octane; C <sub>8</sub>	H <sub>18</sub> ; [111-65-9]	J. Chem. Eng. Data, in press.
(3) 3-Methyl-1-butanol; C <sub>5</sub> H <sub>12</sub> O; [123-51-3]		v. Chem. Eng. Data, in pless.
VARIABLES:		PREPARED BY:
T/K = 298, Solvent composition		W.E. Acree, Jr.
EXPERIMENTAL VALUE t = 25.0 °C	JES <sup>a</sup>	
x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001838

x <sub>3</sub> (s)	<i>x</i> <sub>3</sub>	$x_1$
0.0000	0.0000	0.001838
0.1537	0.1534	0.001814
0.2672	0.2667	0.001728
0.4914	0.4907	0.001488
0.5939	0.5931	0.00134
0.6958	0.6950	0.001199
0.8537	0.8529	0.00095
0.9265	0.9257	0.00084
1.0000	0.9993	0.00072

 $x_{\zeta}^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_{1}$ : mole fraction solubility of the solute; x: 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 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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (3) 3-Methyl-1-butanol; C<sub>5</sub>H<sub>12</sub>O; [123-51-3]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data, in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

+	_	25.	Λ	٥,

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001553
0.1048	0.1046	0.001607
0.2011	0.2008	0.001561
0.3923	0.3918	0.001389
0.4977	0.4971	0.001277
0.5993	0.5986	0.001153
0.7958	0.7951	0.000934
0.8896	0.8889	0.000836
1.0000	0.9993	0.000727

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

## 124 COMPONENTS: ORIGINAL MEASUREMENTS: Zvaigzne, A.I.; Acree, W.E., Jr. (1) Anthracene; C14H10; [120-12-7] (2) Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>; [108-87-2] J. Chem. Eng. Data, in press. (3) 3-Methyl-1-butanol; C<sub>5</sub>H<sub>12</sub>O; [123-51-3] VARIABLES: PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.001649
0.1290	0.1288	0.001709
0.2350	0.2346	0.001633
0.4367	0.4361	0.001422
0.5422	0.5415	0.001299
0.6437	0.6430	0.001153
0.8247	0.8239	0.000923
0.9137	0.9129	0.000821
1.0000	0.9993	0.000727

 $<sup>^{</sup>a}$   $x_{\tau}^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_{\uparrow}$ : mole fraction solubility of the solute; x2: 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 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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 2,2,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]
- (3) 3-Methyl-1-butanol; C<sub>5</sub>H<sub>12</sub>O; [123-51-3]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data, in press.

#### VARTARIES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C	3

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001074
0.1476	0.1474	0.001114
0.2838	0.2835	0.001103
0.4998	0.4993	0.001042
0.6038	0.6032	0.000990
0.6973	0.6966	0.000937
0.8537	0.8530	0.000833
0.9196	0.9189	0.000782
1.0000	0.9993	0.000727

 $<sup>^</sup>a$   $x_3^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) t-Butylcyclohexane;  $C_{10}H_{20}$ ; [3178-22-1]
- (3) 3-Methyl-1-butanol; C<sub>5</sub>H<sub>12</sub>O; [123-51-3]

#### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data, in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

ŧ.	=	25	.0	°C

x <sub>3</sub> (s)	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001978
0.1685	0.1682	0.001938
0.2866	0.2861	0.001843
0.5168	0.5160	0.001545
0.6089	0.6080	0.001400
0.7072	0.7063	0.001217
0.8650	0.8642	0.000944
0.9274	0.9266	0.000852
1.0000	0.9993	0.000727

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]
- (3) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(8)</sup>	<b>x</b> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001274
0.0774	0.0773	0.001469
0.1758	0.1755	0.001608
0.3536	0.3530	0.001827
0.4524	0.4515	0.001917
0.5528	0.5517	0.001979
0.7728	0.7712	0.002101
0.8747	0.8728	0.002138
1.0000	0.9978	0.002160

 $<sup>^</sup>a$   $x_3^{\,(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ mole %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

1.

#### COMPONENTS:

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5]
- (3) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

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

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	$x_1$
0.0000	0.0000	0.001571
0.1018	0.1016	0.001738
0.1925	0.1921	0.001835
0.3897	0.3889	0.002002
0.4808	0.4798	0.002057
0.5865	0.5853	0.002098
0.7841	0.7824	0.002135
0.8958	0.8939	0.002163
1.0000	0.9978	0.002160

 $<sup>^</sup>a$   $x_3^{\,(s)};$  initial mole fraction of binary solvent mixture;  $x_1;$  mole fraction solubility of the solute;  $x_3;$  mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

#### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Anthracene; C14H10; [120-12-7] Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, (2) n-Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9] Fluid Phase Equilibr. 1994, 92, 233-253. (3) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5] PREPARED BY: VARIABLES: T/K = 298, Solvent composition W.E. Acree, Jr. EXPERIMENTAL VALUES t = 25.0 °C x3<sup>(s)</sup> X1 $x_3$ 0.0000 0.001838 0.0000 0.1088 0.001948 0.1090 0.2106 0.002040 0.2110 0.4021 0.4012 0.002138 0.5071 0.5060 0.002169

 $^a$   $x_3^{\,(s)}\colon$  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**

0.002182

0.002175

0.002167

0.002160

#### METHOD: APPARATUS/PROCEDURE

0.6139

0.8015

0.9021

1.0000

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

0.6126

0.7998

0.9001

0.9978

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

# COMPONENTS: (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] (3) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5] VARIABLES: T/K = 298, Solvent composition EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C x<sub>3</sub>(s) x<sub>3</sub> Q.0000 Q.0000 Q.0000 Q.0000 Q.0001553

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	$oldsymbol{x_1}$
0.0000	0.0000	0.001553
0.0815	0.0814	0.001730
0.1521	0.1518	0.001804
0.3128	0.3122	0.001937
0.4106	0.4098	0.002002
0.5153	0.5142	0.002048
0.7254	0.7239	0.002120
0.8499	0.8481	0.002143
1.0000	0.9978	0.002160

 $<sup>^</sup>a$   $x_5^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_1$ : mole fraction solubility of the solute;  $x_3$ : mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

		13
(2) Methylcyclor [108-87-2]	C <sub>14</sub> H <sub>10</sub> ; [120-12-7] nexane; C <sub>7</sub> H <sub>14</sub> ; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]	ORIGINAL MEASUREMENTS:  Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.  Fluid Phase Equilibr. 1994, 92, 233-253.
VARIABLES:  T/K = 298, Solvent composition		PREPARED BY: W.E. Acree, Jr.
EXPERIMENTAL VALUE t = 25.0 °C	TES <sup>a</sup>	
x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	$x_1$
0.0000	0.0000	0.001649
0.0884	0.0882	0.001885
	0.1700	0.001066

x3 <sup>(s)</sup>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001649
0.0884	0.0882	0.001885
0.1712	0.1709	0.001966
0.3497	0.3490	0.002058
0.4438	0.4429	0.002090

0.002119 0.5454 0.5442 0.7623 0.7607 0.002147 0.8752 0.8733 0.002154

0.9978

 $^a$   $x_3^{(s)};$  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**

0.002160

#### METHOD: APPARATUS/PROCEDURE

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 resortions 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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]

- (2) 2,2,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]
- (3) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr. 1994, 92, 233-253.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C

*3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	× <sub>1</sub>
0.0000	0.0000	0.001074
0.1236	0.1234	0.001261
0.2128	0.2125	0.001378
0.4069	0.4062	0.001608
0.5092	0.5083	0.001719
0.6123	0.6112	0.001809
0.8054	0.8038	0.001987
0.8992	0.8973	0.002065
1.0000	0.9978	0.002160

<sup>\*</sup>  $x_{\bar{x}}^{(s)}$ : initial mole fraction of binary solvent mixture;  $x_{\bar{1}}$ : mole fraction solubility of the solute; x3: mole fraction of component 3 in the ternary solution.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.7 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) t-Butylcyclohexane; C<sub>10</sub>H<sub>20</sub>; [3178-22-1]
- (3) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]

#### ORIGINAL MEASUREMENTS:

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

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

#### **VARIABLES:**

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	× <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.001978
0.1124	0.1122	0.002151
0.2170	0.2165	0.002198
0.4191	0.4181	0.002274
0.5221	0.5209	0.002274
0.6185	0.6171	0.002249
0.8152	0.8134	0.002219
0.9127	0.9107	0.002180
1.0000	0.9978	0.002160

 $<sup>^{</sup>a}$   $x_{3}^{\,(s)}\colon$  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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99 %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

## COMPONENTS: (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] (2) 1-Butanol; C4H10O; [71-36-3]

# (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr., in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

:

x <sub>3</sub> (s)	<i>x</i> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.000801
0.1331	0.1330	0.000783
0.2419	0.2417	0.000762
0.4468	0.4465	0.000716
0.5538	0.5534	0.000692
0.6472	0.6468	0.000674
0.8289	0.8284	0.000631
0.9043	0.9037	0.000616
1.0000	0.9994	0.000591

 $<sup>^{</sup>a}$   $x_{3}^{(s)}$ : 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 Attainment of equilibrium temperature. 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 356 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

#### ESTIMATED ERRORS:

- (1) Anthracene; C14H10; [120-12-7]
- (2) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr., in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES

t = 25.0 °C

x <sub>3</sub> (s)	x <sub>3</sub>	<i>x</i> <sub>1</sub>
0.0000	0.0000	0.000585
0.1310	0.1309	0.000586
0.2470	0.2469	0.000584
0.4461	0.4458	0.000586
0.5495	0.5492	0.000586
0.6514	0.6510	0.000588
0.8243	0.8238	0.000593
0.9065	0.9060	0.000592
1.0000	0.9994	0.000591

 $<sup>^</sup>a$   $x_3^{\,(s)};$  initial mole fraction of binary solvent mixture;  $x_1;$  mole fraction solubility of the solute;  $x_3;$  mole fraction of component 3 in the ternary solution.

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

# ESTIMATED ERRORS:

 $T/K: \pm 0.05.$   $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1$  % (relative error).

# COMPONENTS: (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] (2) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0] (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8] VARIABLES: T/K = 298, Solvent composition EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C x<sub>3</sub>(s) x<sub>3</sub> 0.0000 0.000411

x <sub>3</sub> (s)	<b>x</b> <sub>3</sub>	<b>*</b> 1
0.0000	0.0000	0.000411
0.1092	0.1092	0.000436
0.2068	0.2067	0.000449
0.4016	0.4014	0.000478
0.5073	0.5070	0.000497
0.6105	0.6102	0.000516
0.7955	0.7951	0.000553
0.8882	0.8877	0.000572
1.0000	0.9994	0.000591

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

# SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

# ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_3^{(s)}$ :  $\pm$  0.0001.  $x_1$ :  $\pm$  1 % (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr., in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<b>×</b> 1
0.0000	0.0000	0.002160
0.2116	0.2112	0.001873
0.3583	0.3577	0.001655
0.5747	0.5739	0.001322
0.6793	0.6785	0.001145
0.7689	0.7681	0.000996
0.8921	0.8914	0.000782
0.9481	0.9474	0.000688
1.0000	0.9994	0.000591

 $<sup>^{\</sup>rm s}$   $x_3^{\rm (s)};$  initial mole fraction of binary solvent mixture;  $x_1;$  mole fraction solubility of the solute;  $x_3;$  mole fraction of component 3 in the ternary solution.

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

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

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

# ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_3^{(s)}$ :  $\pm$  0.0001.  $x_1$ :  $\pm$  1 % (relative error).

- (1) Anthracene; C14H10; [120-12-7]
- (2) 1-Butanol; C4H10O; [71-36-3]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

# ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr., in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES

t = 25.0 °C

x3 <sup>(s)</sup>	<b>x</b> 3	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.000801
0.1362	0.1361	0.000757
0.2456	0.2454	0.000710
0.4369	0.4366	0.000630
0.5448	0.5445	0.000584
0.6427	0.6423	0.000548
0.8193	0.8189	0.000482
0.9061	0.9057	0.000449
1.0000	0.9996	0.000411

 $<sup>^</sup>a$   $x_3^{\,(s)}\colon$  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 356 nm.

# SOURCE AND PURITY OF MATERIALS:

- (1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) HPLC Grade, 99.8+ %, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

# ESTIMATED ERRORS:

 $T/K: \pm 0.05.$  $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1 \%$  (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]
- (3) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr., in press.

#### VARIABLES:

T/K = 298, Solvent composition

# PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup>

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

x3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<i>*</i> 1
0.0000	0.0000	0.000585
0.1355	0.1354	0.000564
0.2441	0.2440	0.000545
0.4403	0.4401	0.000512
0.5429	0.5426	0.000495
0.6486	0.6483	0.000476
0.8169	0.8165	0.000445
0.9008	0.9004	0.000430
1.0000	0.9996	0.000411

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

## SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

# ESTIMATED ERRORS:

 $T/K: \pm 0.05.$   $x_3^{(s)}: \pm 0.0001.$  $x_1: \pm 1$  (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]
- (3) 2-Butanol; C<sub>4</sub>H<sub>10</sub>O; [15892-23-6]

#### ORIGINAL MEASUREMENTS:

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

Fluid Phase Equilibr., in press.

#### VARIABLES:

T/K = 298, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EIPERIMENTAL VALUES<sup>a</sup>

t = 25.0 °C

*3 <sup>(s)</sup>	<b>x</b> <sub>3</sub>	<b>x</b> <sub>1</sub>
0.0000	0.0000	0.002160
0.1773	0.1770	0.001911
0.3041	0.3036	0.001698
0.5351	0.5344	0.001314
0.6328	0.6321	0.001164
0.7235	0.7228	0.001012
0.8703	0.8696	0.000787
0.9308	0.9302	0.000696
1.0000	0.9994	0.000585

 $<sup>^</sup>a$   $x_3^{(s)}\colon$  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 356 nm.

# SOURCE AND PURITY OF MATERIALS:

- Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.
- (2) 99+ %, anhydrous, Aldrich Chemical Company.
- (3) 99+ %, anhydrous, Aldrich Chemical Company.

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

# ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_3^{(s)}$ :  $\pm$  0.0001.  $x_1$ :  $\pm$  1 % (relative error).

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2.) Acetonitrile; C<sub>2</sub>H<sub>3</sub>N; [75-05-8]
- (3) Water; H<sub>2</sub>O; [7732-18-5]

#### ORIGINAL MEASUREMENTS:

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

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

(Numerical values obtained from L.S. Lee in a private communication.)

#### VARIABLES:

T/K = 296, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup>

t = 23.0 °C

φ <sub>2</sub> <sup>(s)</sup>	$c_1/(\text{mol dm}^{-3})$
0.00	4.16 x 10 <sup>-7</sup>
0.10	$1.30 \times 10^{-6}$
0.20	7.46 x 10 <sup>-6</sup>
0.30	$2.83 \times 10^{-5}$
0.40	$1.94 \times 10^{-4}$
0.50	6.51 x 10 <sup>-4</sup>

 $<sup>^{\</sup>rm a}$   $\phi_2^{\rm (s)};$  initial volume 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 fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrilemethanol-water mobile phase were used in the chromatographic analysis.

# SOURCE AND PURITY OF MATERIALS:

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

# ESTIMATED ERRORS:

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

- (1) Anthracene; C14H10; [120-12-7]
- (2) Methanol; CH,O; [67-56-1]
- (3) Water; H<sub>2</sub>O; [7732-18-5]

#### ORIGINAL MEASUREMENTS:

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

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

(Numerical values obtained from L.S. Lee in a private communication.)

#### VARIABLES:

T/K = 296, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES

#### t = 23.0 °C

φ <sub>2</sub> (s)	$c_1/(\text{mol dm}^{-3})$
0.00	$4.16 \times 10^{-7}$
0.10	$7.41 \times 10^{-7}$
0.20	$1.17 \times 10^{-6}$
0.30	2.88 x 10 <sup>-6</sup>
0.40	$1.02 \times 10^{-5}$
0.50	$4.34 \times 10^{-5}$
0.60	$1.12 \times 10^{-4}$
0.80	$1.03 \times 10^{-3}$
0.90	2.28 x 10 <sup>-3</sup>
1.00	$4.82 \times 10^{-3}$

a  $\phi_2^{(s)}$ : initial volume fraction of binary solvent mixture;  $c_1$ : molar solubility (mol dm<sup>-3</sup>) of the solute.

# **AUXILIARY INFORMATION**

## METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrilemethanol-water mobile phase were used in the chromatographic analysis.

# SOURCE AND PURITY OF MATERIALS:

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

## ESTIMATED ERRORS:

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

- (1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]
- (2) 2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]
- (3) Water; H<sub>2</sub>O; [7732-18-5]

#### ORIGINAL MEASUREMENTS:

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

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

(Numerical values obtained from L.S. Lee in a private communication.)

#### VARIABLES:

T/K = 296, Solvent composition

## PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES<sup>a</sup>

t = 23.0 °C

φ <sub>2</sub> (s)	$c_1/(\text{mol dm}^{-3})$
0.00	$4.16 \times 10^{-7}$
0.10	7.69 x 10 <sup>-7</sup>
0.20	4.57 x 10 <sup>-6</sup>
0.30	$2.47 \times 10^{-5}$
0.40	$1.03 \times 10^{-4}$
0.50	$5.49 \times 10^{-4}$

 $<sup>^{\</sup>rm a}$   $\phi_2^{\rm (s)}\colon$  initial volume 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 fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrilemethanol-water mobile phase were used in the chromatographic analysis.

# SOURCE AND PURITY OF MATERIALS:

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

# ESTIMATED ERRORS:

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

# COMPONENTS: ORIGINAL MEASUREMENTS: Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. (1) Anthracene; C14H10; [120-12-7] (2) Dimethyl sulfoxide; C<sub>2</sub>H<sub>6</sub>OS; [67-68-5] Environ. Sci. Technol. 1990, 24, 639-646. (3) Water; H<sub>2</sub>O; [7732-18-5] (Numerical values obtained from L.S. Lee in a private communication.)

# VARIABLES:

T/K = 296, Solvent composition

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup> t = 23.0 °C

φ <sub>2</sub> (s)	$c_1/(\text{mol dm}^{-3})$
0.00	4.16 x 10 <sup>-7</sup>
0.10	6.06 x 10 <sup>-7</sup>
0.20	2.29 x 10 <sup>-6</sup>
0.30	6.73 x 10 <sup>-6</sup>
0.40	$2.10 \times 10^{-5}$
0.50	5.89 x 10 <sup>-5</sup>
0.60	2.13 x 10 <sup>-4</sup>
0.70	8.86 x 10 <sup>-4</sup>
0.80	$3.76 \times 10^{-3}$
0.90	1.35 x 10 <sup>-2</sup>
1.00	4.23 x 10 <sup>-2</sup>

 $<sup>^{\</sup>rm a}$   $\phi_2^{\rm (s)}\colon$  initial volume 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 fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernature solutions were analyzed by reversed these. tions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile-methanol-water mobile phase were used in the chromatographic analysis.

# SOURCE AND PURITY OF MATERIALS:

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

# ESTIMATED ERRORS:

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

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

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

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) Benz[a]anthracene; C18H12; Lissi, E.A.; Abuin, E.B. [56-55-3] (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 $c_1/(\text{mol dm}^{-3})$ t/°C 20.0 0.0133 AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD: APPARATUS/PROCEDURE Constant temperature bath, centrifuge, thermometer, and an uv/visible spectro-(1) Purity not given, commercial sample of unspecified source, was used as photometer. received. Excess solute and solvent were placed in (2) Purity and chemical source not given, glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. purification procedure not specified. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law. **ESTIMATED ERRORS:**

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

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

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

1-octanol

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

# 

t/°C

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

25.0

0.01563

## 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).

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

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane cyclohexane

- B. Alkenes
- C. Aromatic Hydrocarbons

methylbenzene

D. <u>Esters</u>

ethyl butyrate

- E. Ethers
- F. Haloalkanes and Haloaromatic Hydrocarbons
- G. Alcohols
- H. <u>Ketones</u>

acetone cyclohexanone acetophenone

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo(ghi)perylene; C <sub>22</sub> H <sub>12</sub> ;	Lissi, E.A.; Abuin, E.B.
1 [191-24-2]	· · ·
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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	(mol dm <sup>-3</sup> )
20.0 0.00	012
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:
	$T/K$ : $\pm 2$ . $c_1$ : unknown.

		ORIGINAL MEASUREMENTS:	
(1) Benzo[ghi]perylene; C <sub>22</sub> H <sub>12</sub> ; [191-24-2] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]		Carre, O.R.; Phillips, D.J.; Brennecke, J.F.  Ind. Eng. Chem. Res. 1994, 33, 1255-1262.	
/ARIABLES:		PREPARED BY:	
T/K = Circa 294 (Ambie	ent Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES	-		
t/° C	x <sub>2</sub>	$x_1$	
21.0	0.9999	0.000149	
AUXILIARY INFORMATION			

# METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

# SOURCE AND PURITY OF MATERIALS:

- (1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.
- (2) HPLC Grade, 99+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

# ESTIMATED ERRORS:

T/K:  $\pm$  2 (Compiler).  $x_1$ :  $\pm$  9.5 % (relative error).

	15
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[ghi]perylene; C <sub>22</sub> H <sub>12</sub> ; [191-24-2]	Carre, O.R.; Phillips, D.J.; Brennecke, J.F.
(2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]	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 <sub>2</sub>	×1
21.0 0.9980	0.00204
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
	INFORMATION SOURCE AND PURITY OF MATERIALS:
Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.	(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) ACS Grade, 99 %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.
Attainment of equilibrium was verified by repetitive measurements taken at 24	ESTIMATED ERRORS:
hour intervals.	T/K: ± 2 (Compiler).
	$x_1$ : $\pm 1.4$ % (relative error).

ORIGINAL MEASUREMENTS:		
Carre, O.R.; Phillips, D.J.; Brennecke, J.F.		
Ind. Eng. Chem. Res. 1994, 33, 1355-1362.		
PREPARED BY:		
W.E. Acree, Jr.		
<b>x</b> <sub>1</sub>		
0.00116		
IARY INFORMATION		
SOURCE AND PURITY OF MATERIALS:		
(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.		
(2) 99 %, Aldrich Chemical Company, was used as received.		

152	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[ghi]perylene; C <sub>22</sub> H <sub>12</sub> ; [191-24-2] (2) Acetone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1]	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 <sub>2</sub>	x <sub>1</sub>
21.0 0.9994	0.000634
NITETT TARV	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.	(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) ACS Grade, 99.5 %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.
Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.	ESTIMATED ERRORS:
THE THE VOLUME TO THE TANK THE	$T/K$ : $\pm 2$ (Compiler). $x_1$ : $\pm 0.7$ % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<ol> <li>Benzo[ghi]perylene; C<sub>22</sub>H<sub>12</sub>; [191-24-2]</li> <li>Cyclohexanone; C<sub>6</sub>H<sub>10</sub>O; [108-94-1]</li> </ol>	Carre, O.R.; Phillips, D.J.; Brennecke, J.F.  Ind. Eng. Chem. Res. 1994, 33, 1255-1262.			
VARIABLES:	PREPARED BY:			
T/K = Circa 294 (Ambient Room)	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/° C x <sub>2</sub>	<b>x</b> <sub>1</sub>			
21.0 0.9960	0.00400			
	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.	(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.			
Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis.	(2) 99.8 %, Aldrich Chemical Company, was used as received.			
Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.	ESTIMATED ERRORS:			
	$T/K$ : $\pm 2$ (Compiler). $x_1$ : $\pm 5.1$ % (relative error).			

# COMPONENTS: (1) Benzo[ghi]peryle

(1) Benzo[ghi]perylene; C<sub>22</sub>H<sub>12</sub>;
 [191-24-2]
 (2) Acetophenone; C<sub>8</sub>H<sub>8</sub>O; [98-86-2]

# ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, 33, 1355-1362.

#### VARIABLES:

T/K = Circa 294 (Ambient Room)

#### PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES

t/° C 21.0

x<sub>2</sub>

0.9936

X1

0.00640

#### AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and the solvent evaporated. Residue dissolved in cyclohexane and diluted quantitatively for spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements after 24 hour intervals.

# SOURCE AND PURITY OF MATERIALS:

- 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.
- (2) 99 %, Aldrich Chemical Company, was used as received.

#### ESTIMATED ERRORS:

T/K:  $\pm$  2 (Compiler).  $x_1$ :  $\pm$  4.6 % (relative error).

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

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

	155	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Benzo[a]pyrene; C <sub>20</sub> H <sub>12</sub> ; [50-32-8]	Lissi, E.A.; Abuin, E.B.	
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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	7/(mol dm <sup>-3</sup> )	
20.0	.0034	
AUXILIA	RY INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	<ol> <li>Purity not given, commercial sample of unspecified source, was used as received.</li> </ol>	
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-	ESTIMATED EDDODS:	

polates up to saturation point.

Excess solute and solvent placed in screw-capped test tube and allowed to equilibrate for 3 days with gentle agita-

tion in a constant temperature bath. Samples centrifuged for 30 minutes and concentrations were determined spectro-photometrically. Attainment of equilibrium verified by repetitive measurements

4 days later.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Benzo[a]pyrene; C <sub>20</sub> H <sub>12</sub> ; [50-32-8] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]		Mishra, D.S.; Yalkowsky, S.H.		
		Ind. Eng. Chem. Res., <u>1990</u> , 29, 2278-2283.		
VARIABLES:		PREPARED BY:		
T/K = 296		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>		
23.0	0.9646	0.0354		
	AUXILIX	ARY INFORMATION		
METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, rotator, thermometer, and an uv/visible spectro-		(1) Reagent grade, source not specified, was used as received.		

ESTIMATED ERRORS:

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

T/K:  $\pm$  0.1 (compiler).  $x_1$ :  $\pm$  5 % (relative error; compiler).

ESTIMATED ERRORS:

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

# BIPHENYL SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

# A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
tetracosane
octacosane
cyclohexane
methylcyclohexane
cis-1,2-dimethylcyclohexane
trans-1,2-dimethylcyclohexane
trans-1,4-dimethylcyclohexane

cis-1,3-dimethylcyclohexane decahydronaphthalene

# B. <u>Alkenes</u>

# C. Aromatic Hydrocarbons

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

# D. <u>Esters</u>

# E. Ethers

1,4-dioxane diphenyl ether

# F. Haloalkanes and Haloaromatic Hydrocarbons

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

# G. Alcohols

1-octanol
1-octadecanol

H. <u>Ketones</u>

benzophenone

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

carbon disulfide
pyridine
thiophene
indole
diphenylamine
nitrobenzene
1-octadecanoic acid

J. Binary Solvent Mixtures

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]		Acree, W.E., Jr.		
(2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]		Int. J. Pharm. <u>1984</u> , 18, 47-52.		
VARIABLES:		PREPARED BY:		
T/K = 298		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
t/° C	*2	<i>x</i> <sub>1</sub>		
25.0	0.8767	0.1233		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature ba thermometer, and an ult spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.		
Excess solute and solve glass bottles and allow for several days at con Attainment of equilibri repetitive measurements urated solutions transf coarse filter into tare flasks, weighed and dil	ed to equilibrate stant temperature. um verified by . Aliquots of sat- erred through a d volumetric uted with cyclo-	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.		
hexane. Concentrations spectrophotometrically		ESTIMATED ERRORS:		
		$T/K$ : $\pm 0.05$ . $x_1$ : $\pm 1$ % (relative error).		

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.			
(2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [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 x <sub>2</sub>	x <sub>1</sub>			
25.0 0.876	0.124			
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	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.			
were rotated while bath temperature slowly				
	ESTIMATED ERRORS:  T/K: precision ± 0.1.  x <sub>1</sub> : ± 2 % (relative error; compiler).			

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]		Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.				
		Int. J. Pharm. <u>1986</u> , 31, 225-230.				
VARIABLES:	/ARIABLES: T/K = 303, 308 and 313		PREPARED BY: W.E. Acree, Jr.			
T/K = 303, 3						
EXPERIMENTAL	VALUES					
t/° C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	t/° C	*2	<i>x</i> <sub>1</sub>	
30.0	0.8392	0.1608	40.0	0.7369	0.2631	
35.0	0.7994	0.2006				
		AUXILIARY	INFORMATION	1		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF N	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		store		emical Company, was rular sieves and dis- efore use.		
	r into tared hed and dilut		ESTIMATED	ERRORS:		
flasks, weighed and diluted with cyclo- hexane. Concentrations determined spectrophotometrically at 250 nm.		etermined	T/K: ± 0.	.05.		

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

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

#### ORIGINAL MEASUREMENTS: COMPONENTS: Warner, J.C.; Scheib, R.C.; Svirbely, W.J. (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [92-52-4] J. Chem. Phys. 1934, 2, 590-594. (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5] PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K $x_1$ $x_2$ 299.7 0.860 0.140 0.784 0.216 308.4 0.726 0.274 313.1 316.3 0.665 0.335 319.9 0.591 0.409 322.2 0.532 0.468 0.525 0.475 322.3 0.335 0.665 328.5 330.7 0.284 0.726 332.7 0.197 0.803 333.7 0.194 0.806 334.8 0.164 0.836 335.7 0.143 0.857 337.2 0.108 0.892 339.2 0.066 0.934 341.3 0.028 0.972

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gentle rotation to thoroughly mix contents. Bath temperature was slowly increased and solubility visually determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

#### SOURCE AND PURITY OF MATERIALS:

- Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized three times from alcohol.
- (2) Purity not specified, Eastman Kodak Company, was used as received.

#### ESTIMATED ERRORS:

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

	16	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Lissi, E.A.; Abuin, E.B.	
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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 <sub>1</sub> /	(mol dm <sup>-3</sup> )	
20.0 0.4	15	
AUXILIARY	/ INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	<ol> <li>Purity not given, commercial sample of unspecified source, was used as received.</li> </ol>	
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	(2) Purity and chemical source not given, purification procedure not specified.	
that the dilute solution behavior extra- polates up to saturation point.	ESTIMATED ERRORS:	
	T/K: ± 2.	

omponents:		ORIGINAL	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]		C.L.	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.  Int. J. Pharm. 1986, 31, 225-230.			
VARIABLES:			PREPARED	BY:		
T/K = 303, 3	08 and 313		W.E. Acr	W.E. Acree, Jr.		
EXPERIMENTAL	VALUES		•			
t/° C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	t/° C	×2	<i>×</i> 1	
30.0	0.8250	0.1750	40.0	0.7227	0.2773	

c1: unknown.

# **AUXILIARY INFORMATION**

# METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

# SOURCE AND PURITY OF MATERIALS:

- 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 3 times from methanol.
- (2) 99+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.

### ESTIMATED ERRORS:

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

- (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [120-12-7]
- (2) n-Heptane; C<sub>7</sub>H<sub>16</sub>; [110-54-3]

#### **EVALUATOR:**

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

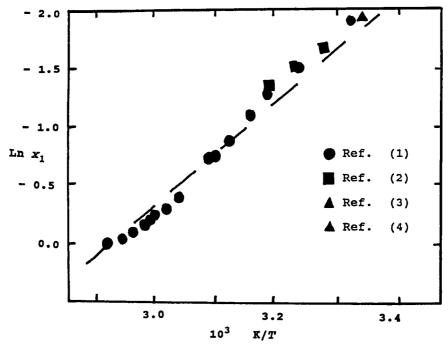
#### CRITICAL EVALUATION:

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

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

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

from experimental values of  $x_1 = 0.1381$  (3) and  $x_1 = 0.138$  (4).



Graphical plot of Ln  $x_1$  versus 1/T

# REFERENCES

- 1. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. J. Chem. Phys. 1934, 2, 590-594.
- Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.
- 3. Acree, W.E., Jr. Int. J. Pharm. 1984, 18, 47-52.
- 4. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.
- 5. Lissi, E.A.; Abuin, E.B. Bol Soc. Chil. Quin. 1981, 26, 19-34.

	100				
COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.				
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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 <sub>2</sub>	<i>x</i> <sub>1</sub>				
25.0 0.862	0.138				
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	(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 <sub>1</sub> versus 1/T graph.	ESTIMATED ERRORS:  T/K: precision ± 0.1.  x <sub>1</sub> : ± 2 % (relative error; compiler).				

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ;	[92-52-4]	Acree, W.E., Jr.				
(2) n-Octane; C <sub>8</sub> H <sub>18</sub> ; [	111-65-9]	Int. J. Pharm. 1984, 18, 47-52.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°C	<b>x</b> <sub>2</sub>	$\mathbf{x_1}$				
25.0	0.8520	0.1480				
A 44	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCE	EDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature I thermometer, and an uspectrophotometer.		(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 cyclo-		(2) Cold Inhal Out & Aldminh Chaminal				
glass bottles and allo for several days at co Attainment of equilibrate repetitive measurement urated solutions transcoarse filter into tar	owed to equilibrate onstant temperature. rium verified by as Aliquots of satserred through a red volumetric	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use				

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

104						
COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ;	[92-52-4]	Chang, W.				
(2) n-Octane; C <sub>8</sub> H <sub>18</sub> ; [	111-65-9]	Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).				
VARIABLES:	<del>-</del>	PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°C	<b>x</b> <sub>2</sub>	× <sub>1</sub>				
25.0	0.853	0.147				
	AUXILIARY	INFORMATION .				
METHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature thermometer.	bath and a precision	(1) Purity, source and purification procedures not specified.				
Mixtures of known con in glass ampoules and temperature to equili were rotated while ba increased. Solubility	placed in constant brate. Samples th temperature slowly	(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.				
noting the temperatur trace of solid solute ubilities at 298 K in experimental values u 1/T graph.	e at which the last disappeared. Sol- terpolated from	ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 2 % (relative error; compiler).				

(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) n-Octane; C <sub>8</sub> H <sub>18</sub> ; [111-65-9]			ORIGINAL MEASUREMENTS:  Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.  Int. J. Pharm. 1986, 31, 225-230.			
T/K = 303, 308 and 313			W.E. Acr	ee, Jr.		
EXPERIMENTAL	VALUES		<del>-</del>			
t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	t/°C	<i>x</i> <sub>2</sub>	<i>*</i> 1	
30.0	0.8164	0.1836	40.0	0.7109	0.2891	
35.0	0.7707	0.2293				
			INFORMATIO			
Constant tem	ATUS/PROCEDUR perature bath and an ultra	E , calorimetric violet/visible	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.			
spectrophoto	meter.	VIOLEC, VIBIBLE				
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.			(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before u			
			ESTIMATED			

OMPONENTS:			ORIGINAL MEASUREMENTS:				
<ul> <li>(1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [92-52-4]</li> <li>(2) Tetracosane; C<sub>24</sub>H<sub>50</sub>; [646-31-1]</li> </ul>			Vitali, G.				
			Int. DATA Ser.	, Ser. A <u>19</u>	<u>34</u> , 94.		
ARIABLES:			PREPARED BY:	<del></del> .			
Temperature			W.E. Acree, Jr	•			
IPERIMENTAL VALUES							
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<b>*</b> 1		
323.8	1.000	0.000	340.3	0.045	0.955		
323.4	0.980	0.020	340.8	0.044	0.956		
323.3	0.972	0.028	341.5	0.022	0.978		
322.8	0.942	0.058	341.9	0.012	0.988		
321.8	0.882	0.118	342.0	0.007	0-993		
320.6	0.804	0.196	342.3	0.000	1.000		
319.8	0.718	0.282					
319.1	0.641	0.359					
318.7	0.623	0.377					
318.0	0.586	0.414					
318.6	0.568	0.432					
319.7	0.544	0.456					
320.8	0.534	0.466					
321.6	0.512	0.488					
323.9	0.477	0.523					
326.0	0.436	0.564					
327.8	0.395	0.605					
328.8	0.383	0.617					
330.5	0.339	0.661					
333.9	0.253	0.747					
336.1	0.183	0.817					
337.4	0.132	0.868					
337.6	0.120	0.880					
338.7	0.087	0.913					
339.5	0.068	0.932					
		AUXILIARV	INFORMATION		<del> </del>		
ETHOD: APPARATUS/PR	OCEDIBE		SOURCE AND PURI	PV OF WATERT	T.S.		

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

- 99 %, Ega, Steinheim, Germany, was used as received.
- (2) 97 %, Baker, Deventer, The Netherlands, was used as received.

# ESTIMATED ERRORS:

T/K: precision  $\pm$  0.25.  $x_1$ :  $\pm$  0.001.

COMPONENTS:	<del></del> 1	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Octacosane; C <sub>28</sub> H <sub>58</sub> ; [630-02-4]		Vitali, G.			
		Int. DATA Ser., Ser. A 1984, 95.			
		1111. Data Bolly Boll is 2201, 101			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	<b>x</b> <sub>2</sub>	x <sub>1</sub>			
334.7	1.000	0.000			
334.5	0.986	0.014			
334.3	0.971	0.029			
334.0	0.952	0.048			
333.5	0.922	0.078			
332.3	0.853	0.147			
331.0	0.767	0.233			
329.5	0.670	0.330			
329.0	0.585	0.415			
327.3	0.505	0.495			
326.2	0.460	0.540			
326.2	0.399	0.601			
331.1	0.306	0.694			
333.4	0.250	0.750			
335.7	0.187	0.813			
337.5	0.128	0.872			
339.9	0.072	0.928			
341.2	0.033	0.967			
341.4	0.023	0.977			
341.9	0.011	0.989			
342.1	0.003	0.997			
342.3	0.000	1.000			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and thermometer.	a precision	(1) 99 %, Ega, Steinheim, Germany, was used as received.			
Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly		(2) 98 %, Ega, Steinheim, Germany, was used as received.			
decreased. Solubility determin noting the temperature at whic	h the first	ESTIMATED ERRORS:			
trace of solid solute appeared	•	$T/K$ : precision $\pm$ 0.25. $x_1$ : $\pm$ 0.001.			

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

COMPONENTS:			ORIGINAL M	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]		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. Acree, Jr.					
EXPERIMENTAL V	ALUES						
T/K	x <sub>2</sub>	<i>*</i> 1	T/K	<b>x</b> <sub>2</sub>	× <sub>1</sub>		
302.35	0.7652	0.2348	326.95	0.3071	0.6929		
310.45	0.6460	0.3540	333.05	0.1748	0.8252		
314.65	0.5681	0.4319					
320.85	0.4384	0.5616					

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) 99.6 %, Eastman Kodak Chemical Company, Rochester, New York, USA, was passed over activated alumina and recrystal-
- 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 MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4	<b>4</b> ]	Chang, W.			
(2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-	82-7]	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	×2	<i>x</i> <sub>1</sub>			
25.0	0.810	0.190			
	AUXILIARY	INFORMATION .			
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and thermometer.	d a precision	(1) Purity, source and purification procedures not specified.			
Mixtures of known concentration glass ampoules and placed temperature to equilibrate. We were rotated while bath tempincreased. Solubility determinates	in constant Samples erature slowly	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.			
noting the temperature at white trace of solid solute disappe	ich the last	ESTIMATED ERRORS:			
ubilities at 298 K interpolate experimental values using ln 1/T graph.	ted from	$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 2 % (relative error; compiler).			

(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]			ORIGINAL MEASUREMENTS:  McLaughlin, E.; Zainal, H.A.  J. Chem. Soc. 1960, 3854-3857.											
							VARIABLES:			PREPARED BY:				
							Temperature			W.E. Acre	e, Jr.			
EXPERIMENTAL '	VALUES													
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	× <sub>2</sub>	× <sub>1</sub>									
299.5	0.7987	0.2013	331.2	0.2186	0.7814									
310.4	0.6503	0.3497												
318.3	0.4978	0.5022												
325.2	0.3473	0.6527												
		AUXILIARY	INFORMATION											
METHOD: APPAR	ATUS/PROCEDUR	દ	SOURCE AND	PURITY OF M	ATERIALS:									
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			(1) 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.											
				ERRORS: ision ± 0.1. 003 (compiler	r).									

- (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [120-12-7]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]

#### **EVALUATOR:**

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

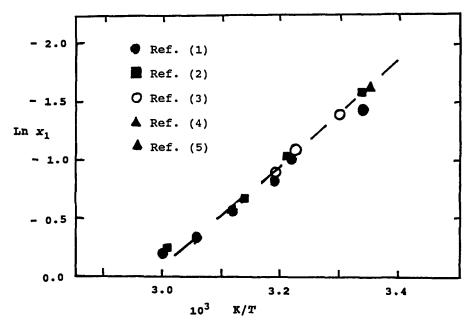
#### CRITICAL EVALUATION:

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

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

$$\text{Ln } x_1 = -4295.7 \ (1/T) + 12.770 \ (r = 0.9975$$

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



Graphical plot of Ln x1 versus 1/T

# REFERENCES

- Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin J. Chem. Eng. Data 1985, 30, 403-409.
- 2. McLaughlin, E.; Zainal, H.A. J. Chem. Soc. 1960, 3854-3857.
- 3. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. Int. J. Pharm. 1986, 31, 225-230.
- 4. Acree, W.E., Jr. Int. J. Pharm. 1984, 18, 47-52.
- 5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:			OPTGTWAT.	WENCHDEWENTS.		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]			ORIGINAL MEASUREMENTS:  Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.  Int. J. Pharm. 1986, 31, 225-230.			
VARIABLES:			PREPARED	BY:		
T/K = 303, 3	008 and 313		W.E. Acr	ee, Jr.		
EXPERIMENTAL	VALUES		+			
t/°C	* <sub>2</sub>	<b>x</b> <sub>1</sub>	t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	
30.0	0.7529	0.2471	40.0	0.6052	0.3948	
35.0	0.6825	0.3175				
		AUXILIARY	INFORMATIO	N	•	
METHOD: APPAR	ATUS/PROCEDUR	.E	SOURCE AN	D PURITY OF M	ATERIALS:	
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			<ol> <li>(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.</li> <li>(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use</li> </ol>			
repetitive measurements. Aliquots of sat- urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclo- hexane. Concentrations determined spectrophotometrically at 250 nm.		ESTIMATED  T/K: ± 0 x1: ± 1		rror).		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.
(2) Methylcyclohexane; C <sub>7</sub> H <sub>14</sub> ; [108-87	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 <sub>2</sub>	x <sub>1</sub>
25.0 0.817	0.183
AU	XILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precitermometer.	ision (1) Purity, source and purification procedures not specified.
Mixtures of known concentrations sea in glass ampoules and placed in cons- temperature to equilibrate. Samples were rotated while bath temperature increased. Solubility determined by	tant Company, USA, was used as received.
noting the temperature at which the trace of solid solute disappeared.	last ESTIMATED ERRORS:
ubilities at 298 K interpolated from experimental values using $\ln x_1$ versu $1/T$ graph.	T/K: precision + 0.1.

	17			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.			
(2) cis-1,2-Dimethylcyclohexane; c <sub>8</sub> H <sub>16</sub> ; [2207-01-4]	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 ×2	× <sub>1</sub>			
25.0 0.805	0.195			
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	(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 <sub>1</sub> versus 1/T graph.	<pre>ESTIMATED ERRORS:  T/K: precision ± 0.1. x<sub>1</sub>: ± 2 % (relative error; compiler).</pre>			

	AUXIL	IARY INFORMATION			
25.0	0.817	0.183			
t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>			
EXPERIMENTAL VALUES					
T/K = 298		W.E. Acree, Jr.			
ARIABLES:		PREPARED BY:			
(2) trans-1,2-Dimethy C <sub>8</sub> H <sub>16</sub> ; [6876-23-9]	lcyclohexane;	Chang, W.  Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ;	[92-52-4]				
COMPONENTS:		ORIGINAL MEASUREMENTS:			

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x<sub>1</sub> versus 1/T graph.

### SOURCE AND PURITY OF MATERIALS:

- Purity, source and purification procedures 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).

l l	ORIGINAL MEASUREMENTS:		
[92-52-4]	Chang, W.  Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).		
ylcyclohexane;			
	PREPARED BY:		
	W.E. Acree, Jr.		
<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>		
0.827	0.173		
AUXILIARY	INFORMATION .		
CEDURE	SOURCE AND PURITY OF MATERIALS:		
bath and a precision	(1) Purity, source and purification proce- dures not specified.		
oncentrations sealed ad placed in constant Librate. Samples what temperature slowly	(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.		
tre at which the last the disappeared. Sol- interpolated from using ln x <sub>1</sub> versus	ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 2 % (relative error; compiler).		
	AUXILIARY  OCEDURE  bath and a precision  concentrations sealed diplaced in constant ibrate. Samples ath temperature slowly y determined by re at which the last ed disappeared. Sol- interpolated from		

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.			
(2) cis-1,4-Dimethylcyclohexane; C <sub>8</sub> H <sub>16</sub> ; [624-29-3]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C × <sub>2</sub>	$x_1$			
25.0 0.818	0.182			
	RY INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.	<ol> <li>Purity, source and purification procedures not specified.</li> </ol>			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowl increased. Solubility determined by	(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. x<sub>1</sub>: ± 2 % (relative error; compiler).</pre>			

	1/3			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.			
(2) cis-1,3-Dimethylcyclohexane; C <sub>8</sub> H <sub>16</sub> ; [638-04-0]	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 ×2	× <sub>1</sub>			
25.0 0.828	0.172			
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	(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 <sub>1</sub> versus 1/T graph.	ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 2 % (relative error; compiler).			

COMPONENTS:			ORIGINAL N	ŒASUREMENTS:	l
(1) Biphenyl	; C <sub>12</sub> H <sub>10</sub> ; [92-	52-4]	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E. Fluid Phase Equilibr. 1989, 44, 305-345.		
(2) Decahydr [91-17-8	onaphthalene; ]	C <sub>10</sub> H <sub>18</sub> ;			
VARIABLES:			PREPARED I	BY:	
Temperature			W.E. Acre	ee, Jr.	
EXPERIMENTAL	VALUES				
T/K	<b>x</b> <sub>2</sub>	<i>*</i> 1	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>
309.0	0.6389	0.3611	328.2	0.4477	0.7385
316.0	0.5260	0.4740			
318.2	0.4820	0.5180			
324.3	0.3594	0.6406			
		AUXILIARY	INFORMATION	1	
ETHOD: APPAR	ATUS/PROCEDUR	lE,	SOURCE AND	PURITY OF M	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		wauke over then (2) 99+ % isome	ee, Wisconsir an activated recrystalliz , Aldrich Ch er ratio of 6	Chemical Company, Mil- A, USA, was passed I alumina column and red from solution. memical Company, having 50.6 % cis and 39.4 % er molecular sieves.	
noting the t		which the last	ESTIMATED	ERRORS:	
rrace or sor	id solute dis	appeared.	7/7	-1-1	

COMPONENTS:			ORIGINAL M	EASUREMENTS:	
<pre>(1) Biphenyl; (2) Benzene;</pre>			McLaughli	n, E.	C.P.; Buehring, K.G.; 985, 30, 403-409.
VARIABLES:			PREPARED B	Y:	
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL V	ALUES				
T/K	x <sub>2</sub>	<b>x</b> <sub>1</sub>	T/K	x <sub>2</sub>	<b>x</b> <sub>1</sub>
307.95	0.5167	0.4833	328.95	0.2289	0.7711
313.85	0.4439	0.5561	333.15	0.1578	0.8422
316.85	0.4068	0.5932			
323.65	0.3103	0.6897			
		AUXILIARY	INFORMATION		
METHOD: 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 noting the temperature at which the last trace of solid solute disappeared.		Roche over lized (2) Gold	ster, New Yo activated al from toluen Label, 99.9+ ny, was used	odak Chemical Company, rk, USA, was passed umina and recrystale e %, Aldrich Chemical as received.	
		~££~~~~	T/K: prec x <sub>1</sub> : ± 0.00	ision $\pm$ 0.1.	

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [	92-52-4]	Chang, W.			
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]  VARIABLES:  T/K = 298		Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).			
		PREPARED BY: W.E. Acree, Jr.			
					XPERIMENTAL VALUES
t/° C	<b>x</b> <sub>2</sub>	x <sub>1</sub>			
25.0	0.619	0.381			
	AUXILIAKI	INFORMATION			
ETHOD: APPARATUS/PROCEI		SOURCE AND PURITY OF MATERIALS:			
ETHOD: APPARATUS/PROCEI Constant temperature ba thermometer.	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature ba	oure  ath and a precision  entrations sealed,  placed in constant rate. Samples  n temperature slowly	SOURCE AND PURITY OF MATERIALS:  (1) Purity, source and purification procedures not specified.			
Constant temperature by thermometer.  Mixtures of known concerninglass ampoules and presenting temperature to equilibute were rotated while bath	entrations sealed a placed in constant rate. Samples a temperature slowly determined by at which the last disappeared. Sol-	SOURCE AND PURITY OF MATERIALS:  (1) Purity, source and purification procedures not specified.  (2) Spectroanalyzed, Eastman Organic Chemical Company, USA, was used as			

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [	92-52-4]	McLaughlin, E.; Zainal, H.A.		
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71	-43-2]	J. Chem. Soc. <u>1959</u> , 863-867.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		<u> </u>		
T/K	<i>x</i> <sub>2</sub>	x <sub>1</sub>		
310.2	0.4882	0.5118		
320.8	0.3522	0.6478		
332.4	0.1805	0.8195		
336.4	0.1084	0.8916		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature between thermometer.	-	(1) Purity not specified, Gesellschaft fur Teerverwertung, 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		(2) "AnalaR", was dried over sodium wire and freshly distilled before use.		
noting the temperature trace of solid solute	at which the last	ESTIMATED ERRORS:		
crace or sorra sorace	allappour ou.	T/K: precision $\pm$ 0.1. x <sub>1</sub> : $\pm$ 0.0003 (compiler).		

COMPONENTS:			ORIGINAL I	ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]			Warner,	Warner, J.C.; Scheib, R.C.; Svirbely, W.J.  J. Chem. Phys. 1934, 2, 590-594.  PREPARED BY:  W.E. Acree, Jr.		
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]		J. Chem.				
VARIABLES:			PREPARED			
Temperature		W.E. Acre				
EXPERIMENTAL '	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	*2	×1	
301.1	0.590	0.410	318.7	0.374	0.626	
316.3	0.415	0.585	322.6	0.323	0.677	
317.5	0.395	0.605	325.5	0.187	0.713	
		AUXIL	IARY INFORMATION	·		
ÆTHOD: APPAR	ATUS/PROCEDU	RE	SOURCE AND	PURITY OF	MATERIALS:	
Constant temperature bath and a precision					fied, Eastman Kodak	

thermometer.

results.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Meas-urements repeated several times to verify

urements repeated several times to verify

# ESTIMATED ERRORS:

hol.

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

(2) Thiophene free, Eastman Kodak Company, was dried over calcium chloride and distilled shortly before use.

Company, Rochester, New York, USA, was recrystallized several times from alco-

### COMPONENTS:

- (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [120-12-7]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

### **EVALUATOR:**

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

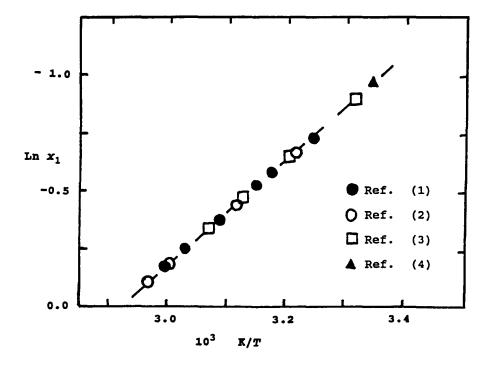
### CRITICAL EVALUATION:

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

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

$$Ln x_1 = -2233.1 (1/T) + 6.5272$$
 (r = 0.9998)

for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is  $x_1 = 0.3819$ , and differs by less than 1 % from experimental value of  $x_1 = 0.381$  (4).



Graphical plot of Ln  $x_1$  versus 1/T

### REFERENCES

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

	17		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.		
(2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]	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 <sub>2</sub>	<i>x</i> <sub>1</sub>		
25.0 0.623	0.377		
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	(2) Reagent Grade, 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 <sub>1</sub> versus 1/T graph.	ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 2 % (relative error; compiler).		

Components:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.
(2) Ethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [100-41-4]	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).
variables:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/° C x <sub>2</sub>	$\mathbf{x_1}$
25.0 0.637	0.363
AUX	ILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
METHOD: APPARATUS/PROCEDURE  Constant temperature bath and a preci- thermometer.	
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constitutemperature to equilibrate. Samples were rotated while bath temperature is	(1) Purity, source and purification procedures not specified.  (2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations seals in glass ampoules and placed in constitution temperature to equilibrate. Samples	sion  (1) Purity, source and purification procedures not specified.  ed (2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.  lowly ast  ESTIMATED ERRORS:

		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Naphthalene; C <sub>10</sub> H <sub>8</sub> ; [91-20-3]		Lee, H.H.; Warner, J.C.		
		J. Am. Chem. Soc. <u>1935</u> , 57, 318-321.		
ARIABLES:		PREPARED BY:		
'emperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>		
353.3	1.000	0.000		
339.3	0.770	0.230		
334.0	0.700	0.300		
334.3	0.697	0.303		
327.5	0.607	0.393		
326.8	0.600	0.400		
322.8	0.551	0.449		
318.6	0.500	0.500		
315.7	0.474	0.526		
314.2	0.459	0.541		
313.0	0.450	0.550		
313.2	0.448	0.552		
312.9	0.447	0.553		
312.8	0.445	0.555		
313.0	0.444	0.556		
315.7	0.427	0.573		
316.1	0.400	0.600		
321.0	0.343	0.657		
	0.300	0.700		
323.5		0.806		
323.5 331.0	0.194			
	0.194	0.898		

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Highest Purity, Eastman Chemicals, was recrystallized.
- (2) Highest Purity, Eastman Chemicals, was recrystallized.

### ESTIMATED ERRORS:

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) 2-Methylnaphthalene; C <sub>11</sub> H <sub>10</sub> ; [91-57-6]  VARIABLES: Temperature		Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.  Int. DATA Ser., Ser. A 1984, 41.  PREPARED BY:			
					W.E. Acree, Jr.
					EXPERIMENTAL VALUES
		T/K	<b>x</b> <sub>2</sub>	$\mathbf{x_1}$	
307.70	1.0000	0.0000			
304.95	0.9071	0.0929			
302.35	0.8127	0.1873			
301.35	0.7649	0.2351			
301.15	0.7489	0.2511			
300.85	0.7328	0.2672			
300.65	0.7167	0.2833			
300.75	0.6974	0.3026			
300.75	0.6844	0.3156			
300.95	0.6780	0.3220			
301.10	0.6682	0.3318			
301.75	0.6519	0.3481			
302.75	0.6356	0.3644			
304.05	0.6193	0.3807			
311.75	0.5203	0.4797			
319.00	0.4196	0.5804			
325.65	0.3173	0.6827			
331.75	0.2133	0.7867			
337.15	0.1075	0.8925			
342.05	0.0000	1.0000			

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

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 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, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.
- (2) Pure Grade, Inst. Chem. Przerobki Wegla, Zabre, Poland, was recrystallized thrice from methanol.

### ESTIMATED ERRORS:

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [92-52-4] Szafranski, A.M.; Wyrzykowska-Stankiewicz, (2) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$ ; [581-42-0] Int. DATA Ser., Ser. A 1984, 42. PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K $x_2$ **x**<sub>1</sub> 383.35 1.0000 0.0000 375.65 0.8483 0.1517 369.45 0.7476 0.2524 351.75 0.4968 0.5032 342.95 0.3969 0.6031 0.7027 331.65 0.2973 329.55 0.2807 0.7193 328.15 0.7276 0.2724 0.7359 327.15 0.2641 328.15 0.2476 0.7524 331.35 0.1979 0.8021 326.95 0.0988 0.9012 342.05 0.0000 1.0000 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Constant temperature bath and a precision (1) Pure Grade, Glovkhimreaktiv, Kharkov, thermometer. USSR, was recrystallized thrice from

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

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

### ESTIMATED ERRORS:

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

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

trace of solid solute disappeared.

results.

Mixtures of known concentrations sealed

noting the temperature at which the last trace of solid solute disappeared. Meas-

urements repeated several times to verify

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

COMPONENTS:	COMPONENTS:		ORIGINAL M	EASUREMENTS:	
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]			Coon, J.E	.; Auwaerter	, J.E.; McLaughlin, E.
(2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2]		Fluid Pha	se Equilibr.	<u>1989</u> , 44, 305-345.	
VARIABLES:		PREPARED E	Y:		
Temperature	Temperature		W.E. Acre	e, Jr.	
EXPERIMENTAL	VALUES		<del> </del>		
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	T/K	× <sub>2</sub>	<i>x</i> <sub>1</sub>
305.6	0.5472	0.4528	322.7	0.3292	0.6708
310.5	0.4940	0.5060	326.9	0.2661	0.7339
314.6	0.4444	0.5556			
319.2	319.2 0.3815 0.6185				
AUXILIARY		INFORMATION			
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		wauke over then (2) 99.6+ store	e, Wisconsin an activated recrystalliz %, Aldrich	chemical Company, Mil- t, USA, was passed alumina column and ed from solution. Chemical Company, was cular sieves to remove	
noting the t	olubility det emperature at	which the last	ESTIMATED	ERRORS:	

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) 1,4-Dioxane; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ; [123-91-1]		ORIGINAL	ORIGINAL MEASUREMENTS: Warner, J.C.; Scheib, R.C.; Svirbely, W.J.			
		Warner,				
		J. Chem.	J. Chem. Phys. <u>1934</u> , 2, 590-594.			
VARIABLES:			PREPARED I	BY:		
Temperature		W.E. Acre	W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	×1	
299.6	0.602	0.398	328.2	0.248	0.752	
305.6	0.543	0.457	330.9	0.204	0.796	
312.5	0.465	0.535	336.6	0.104	0.896	
320.5	0.362	0.638	340.9	0.031	0.969	
326.3	0.275	0.725				
		AUXILI	ARY INFORMATION	N		
METHOD: APPAR	ATUS/PROCEDU	RE	SOURCE AND	D PURITY OF	MATERIALS:	
thermometer.		and a precision	Compa	any, Rochesto estallized so	fied, Eastman Kodak er, New York, USA, was everal times from alco	

# (2) Purity not given, Eastman Kodak Company, was refluxed over metallic sodium and distilled from phosphorous pentoxide. were rotated while bath temperature slowly increased. Solubility determined by ESTIMATED ERRORS:

hol.

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

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Diphenyl ether; C <sub>12</sub> H <sub>10</sub> O; [101-84-8]  VARIABLES: Temperature		Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.  Int. DATA Ser., Ser. A 1984, 43.  PREPARED BY:  W.E. Acree, Jr.				
				EXPERIMENTAL VALUES		
				T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>
				300.00	1.0000	0.0000
294.35	0.8908	0.1092				
289.75	0.7837	0.2163				
286.75	0.7310	0.2690				
286.05	0.7153	0.2847				
289.45	0.6789	0.3211				
301.45	0.5761	0.4239				
310.95	0.4753	0.5247				
318.75	0.3766	0.6234				
325.65	0.2797	0.7203				
331.95	0.1847	0.8153				
337.25	0.0915	0.9085				
341.99	0.0000	1.0000				

### AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

### SOURCE AND PURITY OF MATERIALS:

- Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.
- (2) Pure Grade, Fabryka Odczynnikov Chem., Gliwice, Poland, was distilled before

### ESTIMATED ERRORS:

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]		Chang, W.		
(2) Dichloromethane; CH <sub>2</sub> Cl <sub>2</sub> ; [75-09-2]		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	<i>x</i> <sub>2</sub>	x <sub>1</sub>		
25.0	0.588	0.412		
		INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature bethermometer.	ath and a precision	(1) Purity, source and purification procedures not specified.		
Mixtures of known conc in glass ampoules and temperature to equilib were rotated while bat increased. Solubility	placed in constant rate. Samples h temperature slowly	(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 ubilities at 298 K int	erpolated from	T/K: precision ± 0.1.		
experimental values us 1/T graph.	ing in x <sub>1</sub> versus	$x_1$ : $\pm 2$ % (relative error; compiler).		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]		Chang, W.		
(2) Trichloromethane; CHCl <sub>3</sub> ; [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	<b>x</b> <sub>2</sub>	<b>x</b> 1		
25.0	0.578	0.422		
		INFORMATION		
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:		
•				
Constant temperature bettermometer.	path and a precision	(1) Purity, source and purification procedures not specified.		
	entrations sealed placed in constant orate. Samples the temperature slowly			
Mixtures of known cond in glass ampoules and temperature to equilib were rotated while bat	centrations sealed placed in constant prate. Samples th temperature slowly determined by at which the last	dures not specified. (2) Reagent Grade, Eastman Organic Chem-		

		100
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [9	2-52-4]	Acree, W.E., Jr.
(2) Tetrachloromethane; [56-23-5]	ccl <sub>4</sub> ;	Int. J. Pharm. <u>1984</u> , 18, 47-52.
VARIABLES:	· · · · · · · · · · · · · · · · · · ·	PREPARED BY:
<i>T</i> /K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/° C	x <sub>2</sub>	<b>x</b> <sub>1</sub>
25.0	0.6579	0.3421
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEI	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 cyclo-		(2) 99.8+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.
hexane. Concentrations spectrophotometrically	determined .	ESTIMATED ERRORS:
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).

COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]		4]	Chang, W.  Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).		
		[56-23-5]			
VARIABLES:			PREPARED BY:		
T/K = 298			W.E. Acree, Jr.		
EXPERIMENTAL	VALUES				
t	/° C	× <sub>2</sub>	x <sub>1</sub>		
2	5.0	0.658	0.342		
		AUXILIARY	INFORMATION		
METHOD: APPA	RATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant te	mperature bath an	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 noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x <sub>1</sub> versus 1/T graph.		in constant Samples erature slowly	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.		
		ich the last	ESTIMATED ERRORS:		

100					
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]		ORIGINAL P	MEASUREMENTS	•	
		Warner, J.C.; Scheib, R.C.; Svirbely, W.J.  J. Chem. Phys. 1934, 2, 590-594.			
					VARIABLES:
Temperature	Temperature		W.E. Acre	ee, Jr.	
EXPERIMENTAL	VALUES				
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>
301.3	0.628	0.372	326.8	0.286	0.714
303.9	0.599	0.401	330.6	0.218	0.782
313.2	0.482	0.518	337.5	0.094	0.906
314.5	0.466	0.534	339.2	0.061	0.939
		AUXILIARY	INFORMATION	И	
METHOD: APPAR	METHOD: APPARATUS/PROCEDURE		SOURCE AND	D PURITY OF	MATERIALS:
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.		Compared recry hol.	any, Rochest ystallized s ty not given dried over c	fied, Eastman Kodak er, New York, USA, was everal times from alco- , Eastman Kodak Company, alcium chloride and y before use.	
			ERRORS: cision ± 0.1		

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]  WARIABLES:  Temperature		McLaughlin, E.; Zainal, H.A.			
		J. Chem. Soc. <u>1960</u> , 2485-2488.			
		PREPARED BY: W.E. Acree, Jr.			
					EXPERIMENTAL VALUES
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>			
303.2	0.6037	0.3963			
311.6	0.5054	0.4946			
318.6	0.4002	0.5998			
326.8	0.1721	0.8279			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	OURE	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		<ol> <li>Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.</li> <li>AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.</li> </ol>			
noting the temperature trace of solid solute of	at which the last	ESTIMATED ERRORS:  T/K: precision ± 0.1.  x <sub>1</sub> : ± 0.0003 (compiler).			

### COMPONENTS:

- (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [120-12-7]
- (2) Tetrachloromethane; CCl<sub>4</sub>; [56-23-5]

### **EVALUATOR:**

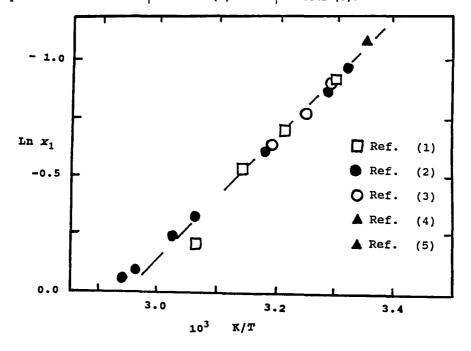
W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
June, 1994

### CRITICAL EVALUATION:

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

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

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



Graphical plot of Ln  $x_1$  versus 1/T

### REFERENCES

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

100				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]  VARIABLES:	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.  Int. J. Pharm. 1986, 31, 225-230.  PREPARED BY:			
T/K = 303, 308 and 313	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x <sub>2</sub> x <sub>1</sub> 30.0 0.6044 0.3956 35.0 0.5426 0.4574	t/°C			
AUXILIAR	Y 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	SOURCE AND PURITY OF MATERIALS:  (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from methanol.  (2) 99.8+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.			
coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.	ESTIMATED ERRORS: $T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1 % (relative error).			

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [9	92-52-4]	Chang, W.			
(2) 1,2-Dibromoethane; [106-93-4]	C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub> ;	Ph.D Dissertation, North Dakota State Uni- versity, North Dakota, USA (1969).			
/ARIABLES:		PREPARED BY:			
T/K = 298		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
t/° C	<b>x</b> <sub>2</sub>	$x_1$			
25.0	0.611	0.389			
· · · · · · · · · · · · · · · · · · ·	AUXILIARY	INFORMATION			
FTHOD. ADDADATIS/DDOCK					
•	DURE	INFORMATION SOURCE AND PURITY OF MATERIALS:			
METHOD: APPARATUS/PROCEI Constant temperature ba thermometer.	DURE				
Constant temperature bathermometer.  Mixtures of known concerning glass ampoules and ptemperature to equilibrate were rotated while bath	entrations sealed claced in constant cate. Samples a temperature slowly	SOURCE AND PURITY OF MATERIALS:  (1) Purity, source and purification proce-			
Constant temperature be thermometer.  Mixtures of known conce in glass ampoules and ptemperature to equilibri	entrations sealed claced in constant cate. Samples a temperature slowly determined by at which the last	(1) Purity, source and purification procedures not specified.  (2) Reagent Grade, Eastman Organic Chem-			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.			
(2) 1,1-Dichloroethane; C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> ; [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 <sub>2</sub>	<i>x</i> <sub>1</sub>			
25.0 0.619	0.381			
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	(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 <sub>1</sub> versus 1/T graph.	ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 2 % (relative error; compiler).			

COMPONENTS:			ORIGINAL MEASUREMENTS:
<ul> <li>(1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [92-52-4]</li> <li>(2) 1,2-Dichloroethane; C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>; [107-06-2]</li> </ul>			Chang, W.
			Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:			PREPARED BY:
T/K = 298	3		W.E. Acree, Jr.
EIPERIMENT	TAL VALUES		
	t/° C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>
	25.0	0.603	0.397
		AUXIL	IARY INFORMATION
METHOD: AP	PARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:

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

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 noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x<sub>1</sub> versus 1/T graph.

- Purity, source and purification procedures not specified.
- (2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.

### ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; (	[92-52-4]	Chang, W.			
(2) Chlorobenzene; C <sub>6</sub> H	<sub>5</sub> cl; [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					
t/° C	<b>x</b> 2	x <sub>1</sub>			
25.0	0.603	0.397			
	AUXILIARY	INFORMATION .			
METHOD: APPARATUS/PROCE	EDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature hetermometer.	oath and a precision	(1) Purity, source and purification procedures not specified.			
Mixtures of known condinglass ampoules and temperature to equilibute rotated while batters and the conditions are the conditions and the conditions are the condition	placed in constant orate. Samples th temperature slowly	(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.			
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x <sub>1</sub> versus 1/T graph.		<pre>ESTIMATED ERRORS:  T/K: precision ± 0.1. x<sub>1</sub>: ± 2 % (relative error; compiler).</pre>			

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) 1,4-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [106-46-7]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS:  Warner, J.C.; Scheib, R.C.; Svirbely, W.J.  J. Chem. Phys. 1934, 2, 590-594.  PREPARED BY:									
						W.E. Acree, Jr.					
						EXPERIMEN	TAL VALUES				
						T/K	<b>x</b> <sub>2</sub>	× <sub>1</sub>	T/K	<b>x</b> 2	<i>×</i> <sub>1</sub>
		300.	9 0.575	0.425	330.6	0.198	0.802				
307.	3 0.504	0.496	334.6	0.141	0.859						
314.	4 0.425	0.575	338.2	0.077	0.923						
323.	0.308	0.692									
		AUXILIARY	INFORMATION	4							
METHOD: A	PPARATUS/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 noting the temperature at which the last trace of solid solute disappeared. Meas-		Compared recry hol. (2) Purit	any, Rocheste ystallized se	fied, Eastman Kodak er, New York, USA, was everal times from alco- , Eastman Kodak Company lved.							
		ESTIMATED	ERRORS:								
urements repeated several times to verify results.		T/K: precision ± 0.1. x <sub>1</sub> : ± 0.002. (compiler).									

### 191 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [92-52-4] Morris, R.E.; Cook, W.A. J. Am. Chem. Soc. 1935, 57, 2403-2406. (2) 1,4-Dichlorobenzene; C6H4Cl2; [106-46-7] PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K $\mathbf{x}_{2}$ ×1 326.4 1.000 0.000 322.6 0.931 0.069 318.2 0.849 0.151 314.4 0.788 0.212 308.4 0.690 0.310 304.0 0.630 0.370 0.425 300.1 0.575 302.6 0.540 0.460 0.480 0.520 308.2 0.560 312.3 0.440 317.3 0.379 0.621 0.708 324.0 0.292 331.9 0.177 0.823 0.106 0.894 336.4 0.950 0.050 339.5 0.000 1.000 342.3 **AUXILIARY INFORMATION**

# METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

### SOURCE AND PURITY OF MATERIALS:

- (1) C.P. grade, Eastman Chemicals, was recrystallized from alcohol to give a melting point temperature of 69.1 °C.
- (2) Purity and chemical source were not specified, was purified by distillation.

### ESTIMATED ERRORS:

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Hexafluorobenzene; C <sub>6</sub> F <sub>6</sub> ; [392-56-3]  VARIABLES:		ORIGINAL MEASUREMENTS:  McLaughlin, E.; Messer, C.E.  J. Chem. Soc., Sect. A 1966, 1106-1110.  PREPARED BY:									
						Temperature			W.E. Acre	e, Jr.	
						EXPERIMENTAL V	ALUES	· · · · · · · · · · · · · · · · · · ·			
						T/K	× <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>
307.45	0.5954	0.4046	331.35	0.2097	0.7903						
310.95	0.5528	0.4472	331.75	0.2025	0.7975						
314.85	0.5031	0.4969	336.55	0.1077	0.8923						
321.30	0.3992	0.6008	337.30	0.0934	0.9066						
326.70	326.70 0.3018 0.6982				•						
		AUXILIARY	INFORMATION	ī							
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:						
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last		(1) Purity not given, Gesellschaft fur Teerverwertung, passed over alumina column, recrystallized and sublimed.									
		(2) Purity not given, Imperial Smelting, Ltd, Avonmouth, Bristol, was dried over anhydrous calcium sulfate.									
		ESTIMATED	ERRORS:								
trace of solid solute disappeared.		T/K: pred x <sub>1</sub> : ± 0.0	ision <u>+</u> 0.1.								

(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]  VARIABLES:  T/K = 298	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	(mol. dm <sup>-3</sup> )			
25.0 0.6				
AUXILIARY	INFORMATION			
Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.  Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.	SOURCE AND PURITY OF MATERIALS:  (1) Highest available commercial purity, specific chemical supplier not given, was used as received.  (2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.  ESTIMATED ERRORS:  T/K: ± 0.1 (compiler).  C1: ± 3 % (relative error; compiler).			

mponents:		ORIGINAL MEASUREMENTS:		
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-5:	2-4}	Berchiesi, G.		
(2) 1-Octadecanol; C <sub>18</sub> H <sub>38</sub> O; [112-92-5]		Int. DATA Ser., Ser. A 1985, 95.		
/ARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES		<u></u>		
T/K	× <sub>2</sub>	x <sub>1</sub>		
331.2	1.0000	0.0000		
330.3	0.9793	0.0207		
329.3	0.9366	0.0634		
328.2	0.8786	0.1214		
327.6	0.8013	0.1987		
325.9	0.7006	0.2994		
324.4	0.5880	0.4120		
325.0	0.5019	0.4981		
329.8	0.3892	0.6108		
332.3	0.3192	0.6808		
334.3	0.2477	0.7523		
336.4	0.1649	0.8351		
338.6	0.0967	0.9033		
340.8	0.0344	0.9656		
342.3	0.0000	1.0000		
		/ TURANUS TAN		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath		(1) 98 %, C. Erba, Milano, Italy, was used		

thermometer.

Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

- as received.
- (2) 99 %, Analytical Reagent, Fluka, St. Gallen, Switzerland, was used as re-ceived.

### ESTIMATED ERRORS:

### 194 ORIGINAL MEASUREMENTS: COMPONENTS: Lee, H.H.; Warner, J.C. (1) Biphenyl; C<sub>12</sub>H<sub>10</sub>; [92-52-4] (2) Benzophenone; C<sub>13</sub>H<sub>10</sub>O; [119-61-9] J. Am. Chem. Soc. 1933, 55, 209-214. PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K $x_2$ $\mathbf{x}_1$ 1.000 0.000 326.0 0.772 0.228 308.2 303.5 0.693 0.307 299.1 0.628 0.372 298.4 0.607 0.393 301.2 0.575 0.425 0.470 305.5 0.530 311.7 0.458 0.542 0.362 0.638 319.3 329.4 0.220 0.780 1.000 342.2 0.000

### 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 noting the temperature at which the last trace of solid solute disappeared.

### SOURCE AND PURITY OF MATERIALS:

- Highest Purity, Eastman Chemicals, was recrystallized from alcohol.
- (2) Highest Purity, Eastman Chemicals, was distilled under reduced pressure.

### ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]	Chang, W.			
(2) Carbon disulfide; CS <sub>2</sub> ; [75-15-0]	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 <sub>2</sub>	x <sub>1</sub>			
25.0 0.631	0.369			
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 were rotated while bath temperature slowly increased. Solubility determined by	(2) Reagent Grade or better, source not specified, was used as received.			
noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x, versus 1/T graph.	ESTIMATED ERRORS:  T/K: precision ± 0.1.  x <sub>1</sub> : '± 2 % (relative error; compiler).			

-52-4]	Wa was s				
•	warner,	Warner, J.C.; Scheib, R.C.; Svirbely, W.J.			
) Carbon disulfide; CS <sub>2</sub> ; [75-15-0]		J. Chem. Phys. <u>1934</u> , 2, 590-594.			
	PREPARED 1	ВҮ:			
	W.E. Acre	e, Jr.			
<i>x</i> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	× <sub>1</sub>		
0.404	317.3	0.405	0.595		
0.498	320.8	0.363	0.637		
0.514	322.7	0.326	0.674		
0.520	324.5	0.306	0.694		
0.553	331.5	0.190	0.810		
	x <sub>1</sub> 0.404 0.498 0.514 0.520	x <sub>1</sub> T/K 0.404 317.3 0.498 320.8 0.514 322.7 0.520 324.5	### PREPARED BY:  W.E. Acree, Jr.  #### T/K		

Constant temperature bath and a precision thermometer.

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

- (1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from alcohol.
- (2) Purity not given, Eastman Kodak Company, was dried over calcium chloride and distilled twice from mercury.

### ESTIMATED ERRORS:

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

COMPONENTS:	OMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]		Choi, P.B.; McLaughlin, E.					
(2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]		Ind. Eng. Chem. Fundam. <u>1983</u> , 22, 46-51.					
VARIABLES:	VARIABLES: Temperature		PREPARED BY:				
Temperature			W.E. Acree, Jr.				
EXPERIMENTAL V	ALUES						
T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	×1		
297.3	0.6258	0.3742	323.7	0.3116	0.6884		
300.9	0.5915	0.4085	331.7	0.1830	0.8170		
307.1	0.5257	0.4743					
312.4	312.4 0.4673 0.5327				•		
		AUXILIARY	INFORMATION	1			
METHOD: APPARA	ATUS/PROCEDUR	6	SOURCE ANI	PURITY OF M	ATERIALS:		
thermometer.	Constant temperature bath and a precision thermometer.		Milwa		mical Company, sin, USA, was used		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.					
noting the to	increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		T/K: prec x <sub>1</sub> : ± 0.0	cision + 0.1.			

(1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> 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	*2	<b>x</b> <sub>1</sub>	T/K	<b>x</b> 2	<b>x</b> <sub>1</sub>
						295.9	0.6149	0.3851	329.5	0.2347	0.7653
						298.4	0.5929	0.4071	334.8	0.1302	0.8698
309.7	0.4782	0.5218									
317.0	0.3940	0.6060									
		AUXILIARY	INFORMATION	ſ							
ETHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:							
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.								
			(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.								
noting the temperature at which the last trace of solid solute disappeared.		T/K: prec x <sub>1</sub> : ± 0.0	ision ± 0.1.								

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Indole; C <sub>8</sub> H <sub>7</sub> N; [120-72-9]  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			<b>x</b> <sub>2</sub>	$x_1$
		326.26	1.0000	0.0000		
317.55	0.8978	0.1022				
310.08	0.8002	0.1998				
306.45	0.7530	0.2470				
301.76	0.6995	0.3005				
301.45	0.6826	0.3174				
304.01	0.6538	0.3462				
308.08	0.6098	0.3902				
312.57	0.5565	0.4435				
318.19	0.4637	0.5363				
323.66	0.3709	0.6291				
328.51	0.2864	0.7136				
335.36	0.1436	0.8564				
343.13	0.0000	1.0000				

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) 99.8 %, Wako Pure Chemical Ind Ltd., was used as received.
- (2) 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

### ESTIMATED ERRORS:

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Indole; C <sub>8</sub> H <sub>7</sub> N; [120-72-9]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS: Szafranski, A.M.; Wyrzykowska-Stankiewicz,		
		Int. DATA Ser., Ser. A 1984, 46.		
		PREPARED BY:		
		W.E. Acree, Jr.		
		EXPERIMENTAL VALUES		
T/K	<b>x</b> <sub>2</sub>	x <sub>1</sub>		
324.95	1.0000	0.0000		
318.75	0.9222	0.0778		
312.65	0.8404	0.1596		
306.45	0.7544	0.2456		
302.05	0.6945	0.3055		
302.70	0.6638	0.3362		
310.95	0.5683	0.4317		
317.65	0.4674	0.5326		
323.85	0.3607	0.6393		
329.75	0.2476	0.7524		
333.90	0.1644	0.8356		
335.75	0.1276	0.8724		
337.00	0.1027	0.8973		
341.99	0.0000	1.0000		
ETHOD: APPARATUS/PROCEI		INFORMATION SOURCE AND PURITY OF MATERIALS:		
Constant temperature bathermometer	ath and a precision	(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from		
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		methanol and zone refined.  (2) Pure Grade, Inst. Chem. Przerobki Wegla, Zabre, Poland, was recrystal- lized thrice from methanol.		
noting the temperature trace of solid solute of		ESTIMATED ERRORS:		
		$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0005.		

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Diphenylamine; C <sub>12</sub> H <sub>11</sub> N; [122-39-4]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS:  Lee, H.H.; Warner, J.C.  J. Am. Chem. Soc. 1933, 55, 209-214.  PREPARED BY:					
					W.E. Acree, Jr.		
					XPERIMENTAL VALUES		——————————————————————————————————————
					T/K	<b>x</b> <sub>2</sub>	x <sub>1</sub>
		326.0	1.000	0.000			
317.7	0.820	0.180					
309.2	0.695	0.305					
306.8	0.646	0.354					
303.5	0.603	0.397					
302.8	0.587	0.417					
304.0	0.565	0.435					
307.3	0.533	0.467					
308.2	0.422	0.478					
312.2	0.477	0.523					
316.9	0.425	0.575					
321.8	0.354	0.646					
326.9	0.268	0.732					
334.1	0.155	0.845					
342.2	0.000	1.000					
BOULDS AND AND A WILL AND A CONTROL OF THE CONTROL		RY INFORMATION					
ETHOD: APPARATUS/PROCED		SOURCE AND PURITY OF MATERIALS:					
Constant temperature ba	-	(1) Highest Purity, Eastman Chemicals, was recrystallized from alcohol.					
Mixtures of known conce in glass ampoules and p temperature to equilibr were rotated while bath	laced in constant ate. Samples temperature slowl	(2) Highest Purity, Eastman Chemicals, was distilled under reduced pressure.					
increased. Solubility d noting the temperature	at which the last	ESTIMATED ERRORS:					
trace of solid solute d	isappeared.	T/K: precision ± 0.1.					

# ESTIMATED ERRORS:

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) Nitrobenzene; C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> ; [98-95-3]  VARIABLES:			ORIGINAL MEASUREMENTS:  Srivastava, R.D.; Gupta, P.D.  J. Indian Chem. Soc. 1967, 44, 960-963.  PREPARED BY:  W.E. Acree, Jr.								
						Temperature					
						EXPERIMENTAL '	VALUES	·		· <u></u>	
						T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>
281.4	0.7858	0.2142				302.2	0.6056	0.3944			
291.4	0.6988	0.3012	305.0	0.5808	0.4192						
296.0	0.6586	0.3414	311.2	0.5093	0.4907						
298.4	0.6399	0.3601									
		AUXILIARY	INFORMATION	1							
METHOD: APPARATUS/PROCEDURE			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 noting the temperature at which the last trace of solid solute disappeared.			y not given, dried and dis	British Drug Houses, tilled.							
		ESTIMATED	ERRORS:								
		T/K: prec x <sub>1</sub> : ± 3 %	ision <u>+</u> 0.1. (relative e	rror, Compiler).							

COMPONENTS:  (1) Biphenyl; C <sub>12</sub> H <sub>10</sub> ; [92-52-4]  (2) 1-Octadecanoic acid; C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> ; [57-11-4]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS:		
		Berchiesi, G.  Int. DATA Ser., Ser. A 1985, 96.  PREPARED BY:		
				W.E. Acree, Jr.
				EXPERIMENTAL VALUES
		T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>
339.3	1.0000	0.0000		
338.7	0.9726	0.0274		
338.0	0.9333	0.0667		
335.5	0.7873	0.2127		
334.4	0.7249	0.2751		
332.4	0.6373	0.3627		
330.7	0.5570	0.4430		
329.9	0.5100	0.4900		
328.3	0.4478	0.5522		
327.7	0.4106	0.5894		
329.3	0.3783	0.6217		
331.0	0.3425	0.6575		
332.8	0.3019	0.6981		
334.6	0.2544	0.7456		
336.4	0.2000	0.8000		
337.7	0.1553	0.8447		
339.2	0.1054	0.8946		
341.3	0.0371	0.9629		
342.3	0.0000	1.0000		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath ar thermometer.	nd a precision	(1) 98 %, C. Erba, Milano, Italy, was used as received.		
Mixtures of known concentrat	ions put	(2) 99 %, Schuchardt, Hohenbrunn, Germany,		

mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

(2) 99 %, Schuchardt, Hohenbrunn, Germany, was used as received.

# ESTIMATED ERRORS:

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

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

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

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) 2,2'-Bipyridine; C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>; [366-18-7] Burgess, J.; Haines, R.I. (2) Methanol; CH<sub>2</sub>O; [67-56-1] Chem. Ind. (London) 1980, 289. (3) Water; H<sub>2</sub>O; [7732-18-5] PREPARED BY: VARIABLES: W.E. Acree, Jr. T/K = 298, Solvent composition

# EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

$\phi_2^{(s)}$	$c_1/(\text{mol dm}^{-3})$
0.00	0.037
0.10	0.063
0.20	0.116
0.30	0.240
0.40	0.60

 $^a$   $\phi_2^{(s)};$  initial volume fraction of binary solvent mixture;  $c_1;$  solubility of the solute expressed in terms of molarity.

# AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.

### SOURCE AND PURITY OF MATERIALS:

- (1) Purity and chemical source not speci-fied, 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).  $\phi_2^{(8)}$ :  $\pm$  0.01 (Compiler).  $c_1$ :  $\pm$  3 % (relative error, Compiler).

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) 2,2'-Bipyridine; C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>; [366-18-7] Burgess, J.; Haines, R.I. (2) Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5] Chem. Ind. (London) 1980, 289. (3) Water; H<sub>2</sub>O; [7732-18-5] **VARIABLES:** PREPARED BY: T/K = 298, Solvent composition W.E. Acree, Jr.

# EXPERIMENTAL VALUES<sup>a</sup> t = 25.0 °C

φ <sub>2</sub> (s)	$c_1/(\text{mol dm}^{-3})$
0.00	0.037
0.10	0.114
0.20	0.240
0.30	0.76

 $^{\rm a}$   $\phi_2^{\rm (s)};$  initial volume fraction of binary solvent mixture;  $c_1;$  solubility of the solute expressed in terms of molarity.

### **AUXILIARY INFORMATION**

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.

### SOURCE AND PURITY OF MATERIALS:

- Purity and chemical source not speci-fied, was recrystallized from aqueous-ethanol.
- (2) Purity and chemical source not speci-fied in paper.
- (3) Purity and chemical source not specified in paper.

### ESTIMATED ERRORS:

 $\begin{array}{l} T/\text{K:} \ \pm \ \text{O.1 (Compiler).} \\ \phi_2^{(s)} \colon \pm \ \text{O.01 (Compiler).} \\ c_1 \colon \pm \ 3 \ \text{\$ (relative error, Compiler).} \end{array}$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2'-Bipyridine; C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> ; [366-18-7]	Burgess, J.; Haines, R.I.
(2) 2-Methyl-2-propanol; C <sub>4</sub> H <sub>10</sub> O; [75-65-0] (3) Water; H <sub>2</sub> O; [7732-18-5]	Chem. Ind. (London) <u>1980</u> , 289.
VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.
EXPERIMENTAL VALUES <sup>a</sup> t = 25.0 °C	
ф.(s)	G.//mol dm <sup>-3</sup> )

φ <sub>2</sub> (s)	$c_1/(\text{mol dm}^{-3}$
0.00	0.037
0.05	0.078
0.10	0.120
0.15	0.195
0.20	0.33
0.25	0.92

 $<sup>^{</sup>a}$   $\phi_{2}{}^{(s)};$  initial volume fraction of binary solvent mixture;  $c_{1};$  solubility of the solute expressed in terms of molarity.

# AUXILIARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.

### SOURCE AND PURITY OF MATERIALS:

- 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).

### BUCKMINSTERFULLERENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

### A. Saturated Hydrocarbons (including cycloalkanes)

- n-pentane
- n-hexane
- n-octane
- n-decane
- n-dodecane

# B. Alkenes

### C. Aromatic Hydrocarbons

benzene

methylbenzene

ethylbenzene

n-propylbenzene

iso-propylbenzene

n-butylbenzene

sec-butylbenzene

t-butylbenzene

1,2-dimethylbenzene

1,3-dimethylbenzene

1,4-dimethylbenzene

1,2,3-trimethylbenzene

1,2,4-trimethylbenzene

1,3,5-trimethylbenzene

1,2,3,4-tetramethylbenzene

1,2,3,5-tetramethylbenzene

1,2,3,4-tetrahydronaphthalene

1-methylnaphthalene

### D. Esters

## E. Ethers

1,4-dioxane methoxybenzene

### F. Haloalkanes and Haloaromatic Hydrocarbons

dichloromethane

trichloromethane

tetrachloromethane

1,2-dibromoethane

tetrachloroethylene

1,1,2,2-tetrachloroethane

bromobenzene

chlorobenzene

- 1,2-dibromobenzene
- 1,3-dibromobenzene
- 1,2-dichlorobenzene
- 1,3-dichlorobenzene
- 1,2,4-trichlorobenzene

fluorobenzene

iodobenzene

1-bromo-2-methylnaphthalene

# G. Alcohols

2-hydroxymethylbenzene

# H. <u>Ketones</u>

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

carbon disulfide
benzonitrile
nitrobenzene
pyridine
quinoline
thiophene
2-methylthiophene
tetrahydrothiophene

# J. Binary Solvent Mixtures

208	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) n-Pentane; C <sub>5</sub> H <sub>12</sub> ; [109-66-0]	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	•
$t/^{\circ}C$ $c_{1}/(\text{mol dm}^{-3})$	
30.0 5.55 x 10 <sup>-6</sup>	
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.  (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.
	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1. $c_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) n-Pentane; C <sub>5</sub> H <sub>12</sub> ; [109-66-0]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C ×1	
22 8	x 10 <sup>-7</sup>
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.  Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentra-	grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as
tions determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile	ESTIMATED ERRORS:
phase was used.	T/K: ± 3.

	208
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
30.0 5.55 x 10 <sup>-5</sup>	
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.  (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.
	ESTIMATED ERRORS:
	$T/K$ : $\pm 0.1$ . $c_1$ : $\pm 3$ % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. 1993, 97, 3379-3383.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	<b>x</b> <sub>1</sub>	
22	7.3 x 10 <sup>-6</sup>	
	ARY INFORMATION  SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE  High performance liquid chromatograph system equipped with an ultraviolet det tor aned integrator.	(1) Graphite soot obtained by passing a ac discharge between spectroscopic grade graphite, and sample purified	
Excess solute and solvent placed in 1-dram glass bottle and allowed to equi for 24 hours at ambient room temperatur with agitation. Saturated solution was filtered through a 0.45 micrometer poly (tetrafluoroethylene) filter. Concentr tions determined via HPLC with uv detec	(2) Reagent grade, 99 % (or better), cheical source not given, used as recefrom manufacturer.	na em-

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>50</sub> ; [99685-96-8] (2) n-Octane; C <sub>8</sub> H <sub>18</sub> ; [111-65-9]	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
30.0 3.4	7 x 10 <sup>-5</sup>
	INFORMATION
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.  (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.
proper and a monamor	ESTIMATED ERRORS:  T/K: + 0.1.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) n-Decane; C <sub>10</sub> H <sub>22</sub> ; [124-18-5]	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.	
VARIABLES:	PREPARED BY:	
T/K = 303	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	$c_1/(\text{mol dm}^{-3})$	
30.0	9.71 x 10 <sup>-5</sup>	
A	UXILIARY INFORMATION	

# METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.
- (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

# ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C<sub>60</sub>;     [99685-96-8] (2) n-Decane; C<sub>10</sub>H<sub>22</sub>; [124-18-5]</pre>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. 1993, 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

t/°C

 $x_1$ 

22

1.9 x 10<sup>-5</sup>

#### AUXILIARY INFORMATION

## METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

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

ORIGINAL MEASUREMENTS:
Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
PREPARED BY:
W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/°C

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

30.0

 $1.26 \times 10^{-4}$ 

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.
- (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

# ESTIMATED ERRORS:

212	
COMPONENTS:  (1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	ORIGINAL MEASUREMENTS:  Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.  J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
30.0 2.00 x 10 <sup>-3</sup>	
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	<ul> <li>(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.</li> <li>(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.</li> </ul>
	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1. $c_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	<b>x</b> ,

 $2.1 \times 10^{-4}$ 

AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

22

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

## ESTIMATED ERRORS:

	213
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ;	Scrivens, W.A.; Tour, J.M.
[99685-96-8] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 2.1	x 10 <sup>-3</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007 \text{ mol dm}^{-3}$ .

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Buckminsterfullerene; C<sub>60</sub>;         [99685-96-8]</li> <li>Methylbenzene; C<sub>7</sub>H<sub>8</sub>; [108-88-3]</li> </ol>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$c_1/(mol dm^{-3})$	
30.0 2.98 x 10 <sup>-3</sup>	
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.  (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

214	
COMPONENTS:  (1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]  VARIABLES:	ORIGINAL MEASUREMENTS:  Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.  J. Phys. Chem. 1993, 97, 3379-3383.  PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	
22 4.0	x 10 <sup>-4</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.  Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a	<ul> <li>(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.</li> <li>(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.</li> </ul>
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS: $T/K$ : $\pm$ 3. $x_1$ : $\pm$ 8 % (relative error; compiler).

Components:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	/(mol dm <sup>-3</sup> )
22 4.	0 x 10 <sup>-3</sup>
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	PONTMATTE BEDONG.

ESTIMATED ERRORS:

T/K:  $\pm$  3 (Compiler),  $c_1$ :  $\pm$  0.0007 mol dm<sup>-3</sup>.

	<b>~</b> 11
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) Ethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [100-41-4]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 3.6	x 10 <sup>-3</sup>
	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 3 (Compiler). $c_1$ : $\pm$ 0.0007 mol dm <sup>-3</sup> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) n-Propylbenzene; C <sub>9</sub> H <sub>12</sub> ; [103-65-1]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

 $t/^{\circ}C$   $c_{1}/(\text{mol dm}^{-3})$ 22  $2.1 \times 10^{-3}$ 

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45  $\mu m$  HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

# SOURCE AND PURITY OF MATERIALS:

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

#### ESTIMATED ERRORS:

T/K:  $\pm$  3 (Compiler).  $c_1$ :  $\pm$  0.0007 mol dm<sup>-3</sup>.

NTS: our, J.M. em. Commun. <u>1993</u> , 1207-
·
em. Commun. <u>1993</u> , 1207-
OF MATERIALS:
emical source were not
paper.
emical source were not paper.
r). lm <sup>-3</sup> .
• E

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) n-Butylbenzene; C <sub>10</sub> H <sub>14</sub> ; [104-51-8]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
	6 x 10 <sup>-3</sup>
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.  Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	<ul><li>(1) Purity and chemical source were not given in the paper.</li><li>(2) Purity and chemical source were not given in the paper.</li></ul>
residue.	ESTIMATED ERRORS: $T/K$ : $\pm$ 3 (Compiler). $c_1$ : $\pm$ 0.0007 mol dm <sup>-3</sup> .

_	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) sec-Butylbenzene; C <sub>10</sub> H <sub>14</sub> ; [135-98-8]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
±/°C	(mol dm <sup>-3</sup> )
22 1.5	5 x 10 <sup>-3</sup>
	<del></del>
AUXILIARY	! INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	
	ESTIMATED ERRORS:

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

t/°C

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

22

 $1 \times 10^{-3}$ 

# **AUXILIARY INFORMATION**

# METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45  $\mu m$  HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

# SOURCE AND PURITY OF MATERIALS:

- (1) Purity and chemical source were not given in the paper.
- (2) Purity and chemical source were not given in the paper.

# ESTIMATED ERRORS:

T/K:  $\pm$  3 (Compiler).  $c_1$ :  $\pm$  0.0007 mol dm<sup>-3</sup>.

OMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]</li> <li>(2) 1,2-Dimethylbenzene; C<sub>8</sub>H<sub>10</sub>; [95-47-6]</li> </ul>	Scrivens, W.A.; Tour, J.M.  J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207-1209.
ARIABLES:	PREPARED BY:
F/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 1.2	x 10 <sup>-2</sup>
AUXILIARY ETHOD: APPARATUS/PROCEDURE	INFORMATION SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.  Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	<ul><li>(1) Purity and chemical source were not given in the paper.</li><li>(2) Purity and chemical source were not given in the paper.</li></ul>
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007$ mol dm <sup>-3</sup> .

Components:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,3-Dimethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [108-38-3]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
variables:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 1.9	× 10 <sup>-3</sup>
METHOD: APPARATUS/PROCEDURE  Analytical balance and centrifuge.  Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source were not given in the paper.  (2) Purity and chemical source were not given in the paper.
about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.	ESTIMATED ERRORS:  T/K: ± 3 (Compiler).  c <sub>1</sub> : ± 0.0007 mol dm <sup>-3</sup> .
	$c_4$ : + 0.0007 mol dm <sup>3</sup> .

	<b>~</b> 1.
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,4-Dimethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [106-42-3]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	$(mol dm^{-3})$
22 8.2	× 10 <sup>-3</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 3 (Compiler). $c_1$ : $\pm$ 0.0007 mol dm <sup>-3</sup> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,2,3-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [526-73-8]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

t/°C

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

22

 $6.5 \times 10^{-3}$ 

## AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

# SOURCE AND PURITY OF MATERIALS:

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

## ESTIMATED ERRORS:

T/K:  $\pm$  3 (Compiler).  $c_1$ :  $\pm$  0.0007 mol dm<sup>-3</sup>.

220		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ;	Scrivens, W.A.; Tour, J.M.	
[99685-96-8] (2) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
±/°C	(mol dm <sup>-3</sup> )	
22 2.4	2.48 x 10 <sup>-2</sup>	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007$ mol dm <sup>-3</sup> .	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) 1,3,5-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [108-67-8]	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.  J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.

t/°C

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

30.0

 $1.38 \times 10^{-3}$ 

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.
- (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

#### ESTIMATED ERRORS:

	22	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.	
(2) 1,3,5-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [108-67-8]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.	
variables:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C x <sub>1</sub>		
22 3.1	x 10 <sup>-4</sup>	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.  Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a	<ul> <li>(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.</li> <li>(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.</li> </ul>	
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:  T/K: ± 3.  x <sub>1</sub> : ± 8 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ;	Scrivens, W.A.; Tour, J.M.	
[99685-96-8] (2) 1,3,5-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [108-67-8]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	$c_1/(\text{mol dm}^{-3})$	
22 2.4	x 10 <sup>-3</sup>	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	T/K: ± 3 (Compiler). c <sub>1</sub> : ± 0.0007 mol dm <sup>-3</sup> .	

222	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,2,3,4-Tetramethylbenzene; C <sub>10</sub> H <sub>14</sub> ; [488-23-3]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 8.0	× 10 <sup>-2</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007 \text{ mol dm}^{-3}$ .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) 1,2,3,5-Tetramethylbenzene; C <sub>10</sub> H <sub>14</sub> ; [527-53-7]  VARIABLES:  T/K = Circa 295 (Ambient Room)  EXPERIMENTAL VALUES  t/°C C <sub>1</sub> /	Scrivens, W.A.; Tour, J.M.  J. Chem. Soc., Chem. Commun. 1993, 1207-1209.  PREPARED BY:  W.E. Acree, Jr.  (mol dm <sup>-3</sup> )
22 2.89 x 10 <sup>-2</sup>	
Analytical balance and centrifuge.  Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated	<ul><li>(1) Purity and chemical source were not given in the paper.</li><li>(2) Purity and chemical source were not given in the paper.</li></ul>
oil bath to facilitate solvent evapora- tion. Concentrations determined gravi- metrically from the weight of the solid residue.	ESTIMATED ERRORS:  T/K: ± 3 (Compiler), c <sub>1</sub> : ± 0.0007 mol dm <sup>-3</sup> .

#### COMPONENTS:

- (1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]
- (2) 1,2,3,4-Tetrahydronaphthalene; C<sub>10</sub>H<sub>12</sub>; [119-64-2]

#### ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, 97, 3379-3383.

#### VARIABLES:

T/K = Circa 295 (Ambient Room)

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/°C

¥.

22

 $3.1 \times 10^{-5}$ 

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

## SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

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

# COMPONENTS:

- (1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]
- (2) 1-Methylnaphthalene; C<sub>11</sub>H<sub>10</sub>; [90-12-0]

# ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, 97, 3379-3383.

#### VARIABLES:

T/K = Circa 295 (Ambient Room)

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/°C

 $x_1$ 

22

6.8 x 10<sup>-5</sup>

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
3000	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) i-Methylnaphthalene; C <sub>11</sub> H <sub>10</sub> ; [90-12-0]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$t/^{\circ}C$ $G_{1}/(\text{mol dm}^{-3})$	
22 4.6	1 x 10 <sup>-2</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007$ mol dm <sup>-3</sup> .

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Buckminsterfullerene; C<sub>60</sub>;      [99685-96-8] (2) 1,4-Dioxane; C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>; [123-91-1]</pre>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.	
VARIABLES:	PREPARED BY:	
T/K = 303	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	(mol dm <sup>-3</sup> )	
30.0 5.6	5.69 x 10 <sup>-5</sup>	
	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.  (2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.	
	ESTIMATED ERRORS:	
	$T/K$ : $\pm 0.1$ . $c_1$ : $\pm 3$ % (relative error; compiler).	

#### COMPONENTS:

- (1) Buckminsterfullerene; CAO; [99685-96-8]
- (2) Methoxybenzene; C7H8O; [100-66-3]

## ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.;

J. Phys. Chem. 1993, 97, 3379-3383.

#### VARIABLES:

T/K = Circa 295 (Ambient Room)

## PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/°C

x,

22

 $8.4 \times 10^{-4}$ 

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

T/K:  $\pm$  3.

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

# COMPONENTS:

- (1) Buckminsterfullerene; C60;
- [99685-96-8]
  (2) Dichloromethane; CH<sub>2</sub>Cl<sub>2</sub>; [75-09-2]

# ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.

#### VARIABLES:

T/K = 303

#### PREPARED BY:

W.E. Acree. Jr.

# EXPERIMENTAL VALUES

t/°C

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

30.0

 $3.52 \times 10^{-4}$ 

# **AUXILIARY INFORMATION**

## METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with-and the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

## SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.
- (2) HPLC grade or AR grade solvent, chem-ical source not given, aromatic impuri-ties removed by chromatography if necessary.

## ESTIMATED ERRORS:

# 226 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Buckminsterfullerene; C<sub>60</sub>; Ruoff, R.S.; Tse, D.S.; Malhotra, R.; [99685-96-8] Lorents, D.C. (2) Dichloromethane; CH<sub>2</sub>Cl<sub>2</sub>; [75-09-2] J. Phys. Chem. 1993, 97, 3379-3383. VARIABLES: PREPARED BY: T/K = Circa 295 (Ambient Room) W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C ×1 $2.7 \times 10^{-5}$ 22 **AUXILIARY INFORMATION**

## METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### **ESTIMATED ERRORS:**

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/ºC

 $\boldsymbol{x_1}$ 

22

 $2.2 \times 10^{-5}$ 

# **AUXILIARY INFORMATION**

# METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer. Reported to contain 1 % ethanol as a stabilizer.

# ESTIMATED ERRORS:

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

	22.
COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Buckminsterfullerene; C<sub>60</sub>;         [99685-96-8]</li> <li>(2) Tetrachloromethane; CCl<sub>4</sub>; [56-23-5]</li> </ul>	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
30.0 6.2	00 x 10 <sup>-4</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.  Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.	<ol> <li>(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.</li> <li>(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.</li> </ol>
	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1. $c_i$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Buckminsterfullerene; C<sub>60</sub>;     [99685-96-8] (2) Tetrachloromethane; CCl<sub>k</sub>; [56-23-5]</pre>	
•	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	x <sub>1</sub>
22 4.0 x 10 <sup>-5</sup>	
AUXII METHOD: APPARATUS/PROCEDURE	LIARY INFORMATION
High performance liquid chromatograph system equipped with an ultraviolet det tor aned integrator.	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina
system equipped with an ultraviolet det	(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.  (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

228		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) 1,2-Dibromoethane; C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub> ; [106-93-4]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C x <sub>1</sub>		
22 6.0	x 10 <sup>-5</sup>	
AUXILIARY INFORMATION		
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.  Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a	<ul> <li>(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.</li> <li>(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.</li> </ul>	
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]</li> <li>(2) Tetrachloroethylene; C<sub>2</sub>Cl<sub>4</sub>; [127-18-4]</li> </ul>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

T/K:  $\pm$  3.

22

 $1.7 \times 10^{-5}$ 

# **AUXILIARY INFORMATION**

## METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

## SOURCE AND PURITY OF MATERIALS:

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

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

# ESTIMATED ERRORS:

# ORIGINAL MEASUREMENTS: COMPONENTS: Ruoff, R.S.; Tse, D.S.; Malhotra, R.; (1) Buckminsterfullerene; Cso; [99685-96-8] (2) 1,1,2,2-Tetrachloroethane; C<sub>2</sub>H<sub>2</sub>Cl<sub>4</sub>; Lorents, D.C. J. Phys. Chem. 1993, 97, 3379-3383. [79-34-5] PREPARED BY: VARIABLES: W.E. Acree, Jr. T/K = Circa 295 (Ambient Room) EXPERIMENTAL VALUES t/°C $7.7 \times 10^{-4}$ 22

#### **AUXILIARY INFORMATION**

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

## SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Buckminsterfullerene; C<sub>60</sub>;         [99685-96-8]</li> <li>Bromobenzene; C<sub>6</sub>H<sub>5</sub>Br; [108-86-1]</li> </ol>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

# EXPERIMENTAL VALUES

t/°C

x,

22

4.8 x 10<sup>-4</sup>

## AUXILIARY INFORMATION

## METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

## SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

# ESTIMATED ERRORS:

230	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ;	Scrivens, W.A.; Tour, J.M.
[99685-96-8] (2) Bromobenzene; C <sub>6</sub> H <sub>5</sub> Br; [108-86-1]	J. Chem. Soc., Chem. Commun. 1993, 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
3.9	x 10 <sup>-3</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	T/K: ± 3 (Compiler). $c_1$ : ± 0.0007 mol dm <sup>-3</sup> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Buckminsterfullerene; C<sub>60</sub>;         [99685-96-8]</li> <li>Chlorobenzene; C<sub>6</sub>H<sub>5</sub>C1; [108-90-7]</li> </ol>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. 1993, 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	× <sub>1</sub>
22	9.9 x 10 <sup>-4</sup>

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

# ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.	
(2) Chlorobenzene; C <sub>6</sub> H <sub>5</sub> Cl; [108-90-7]	J. Chem. Soc., Chem. Commun. 1993, 1207- 1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	$c_1/(\text{mol dm}^{-3})$	
22 7.9	x 10 <sup>-3</sup>	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.	
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	$T/K: \pm 3$ (Compiler). $c_1: \pm 0.0007 \text{ mol dm}^{-3}$ .	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) 1,2-Dibromobenzene; C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub> ; [583-53-9]	Scrivens, W.A.; Tour, J.M.  J. Chem. Soc., Chem. Commun. 1993, 1207-1209.	
VARIABLES:	PREPARED BY:	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.	
EIPERIMENTAL VALUES		
t/°C	$c_1/(\text{mol dm}^{-3})$	
22 1.9	x 10 <sup>-2</sup>	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Analytical balance and centrifuge.  Excess solute and solvent allowed to	(1) Purity and chemical source were not given in the paper.	
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 \(\mu\) MPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.	
residue.	ESTIMATED ERRORS:	
	T/K: ± 3 (Compiler) 3.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,3-Dibromobenzene; C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub> ; (108-36-1)	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
ARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
XPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 1.9	x 10 <sup>-2</sup>
AUXILIARY	INFORMATION
ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared	(2) Purity and chemical source were not given in the paper.
vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.	
	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007$ mol dm <sup>-3</sup> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) 1,2-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [95-50-1]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. 1993, 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.

t/°C

 $x_1$ 

22

5.3 x 10<sup>-5</sup>

# AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

# ESTIMATED ERRORS:

	200
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,2-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [95-50-1]	J. Chem. Soc., Chem. Commun. 1993, 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 3.4	1 x 10 <sup>-2</sup>
	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007 \text{ mol dm}^{-3}$ .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) 1,3-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [541-73-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 3.3	x 10 <sup>-3</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.  Excess solute and solvent allowed to	(1) Purity and chemical source were not given in the paper.
equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007$ mol dm <sup>-3</sup> .

233

# COMPONENTS:

- (1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]
- (2) 1,2,4-Trichlorobenzene; C<sub>6</sub>H<sub>3</sub>Cl<sub>3</sub>; [120-82-1]

# ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, 97, 3379-3383.

#### VARIABLES:

T/K = Circa 295 (Ambient Room)

#### PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/°C

*x*<sub>1</sub>

22

 $1.5 \times 10^{-5}$ 

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

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

#### COMPONENTS:

- (1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]
- (2) 1,2,4-Trichlorobenzene; C<sub>6</sub>H<sub>3</sub>Cl<sub>3</sub>; [120-82-1]

#### ORIGINAL MEASUREMENTS:

- Scrivens, W.A.; Tour, J.M.
- J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

# VARIABLES:

T/K = Circa 295 (Ambient Room)

# PREPARED BY:

W.E. Acree, Jr.

# EXPERIMENTAL VALUES

t/°C

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

22

 $1.44 \times 10^{-2}$ 

# AUXILIARY INFORMATION

## METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45  $\mu \rm m$  HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

## SOURCE AND PURITY OF MATERIALS:

- (1) Purity and chemical source were not given in the paper.
- (2) Purity and chemical source were not given in the paper.

# ESTIMATED ERRORS:

T/K:  $\pm 3$  (Compiler).  $c_1$ :  $\pm 0.0007$  mol dm<sup>-3</sup>.

	235
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) Fluorobenzene; C <sub>6</sub> H <sub>5</sub> F; [462-06-6]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C ×1	
22 7.8	x 10 <sup>-5</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.  Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a	<ol> <li>Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.</li> <li>Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.</li> </ol>
dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:  T/K: ± 3.  x <sub>1</sub> : ± 8 % (relative error; compiler).

COMPONENTS:  (1) Buckminsterfullerene; C <sub>60</sub> ;  [99685-96-8] (2) Fluorobenzene; C <sub>6</sub> H <sub>5</sub> F; [462-06-6]  VARIABLES:  T/K = Circa 295 (Ambient Room)	ORIGINAL MEASUREMENTS:  Scrivens, W.A.; Tour, J.M.  J. Chem. Soc., Chem. Commun. 1993, 1207-1209.  PREPARED BY:  W.E. Acree, Jr.
-	/(mol dm <sup>-3</sup> ) 7 x 10 <sup>-3</sup>
AUXILIAR	Y INFORMATION
Analytical balance and centrifuge.  Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravi-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source were not given in the paper.  (2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K:  $\pm$  3 (Compiler).  $c_1$ :  $\pm$  0.0007 mol dm<sup>-3</sup>.

residue.

230	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Iodobenzene; C <sub>6</sub> H <sub>5</sub> I; [591-50-4]	Scrivens, W.A.; Tour, J.M.  J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EIPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 2.9	ж 10 <sup>-3</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007 \text{ mol dm}^{-3}$ .

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]</li> <li>(2) 1-Bromo-2-methylnaphthalene; C<sub>11</sub>H<sub>9</sub>Br; [2586-62-1]</li> </ul>	Scrivens, W.A.; Tour, J.M.  J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 4.83	3 x 10 <sup>-2</sup>
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.  Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	<ul><li>(1) Purity and chemical source were not given in the paper.</li><li>(2) Purity and chemical source were not given in the paper.</li></ul>
residue.	ESTIMATED ERRORS: $T/K$ : $\pm$ 3 (Compiler). $c_1$ : $\pm$ 0.0007 mol dm <sup>-3</sup> .

#### 237 COMPONENTS: ORIGINAL MEASUREMENTS: Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. (1) Buckminsterfullerene; CAO; [99685-96-8] (2) 2-Hydroxymethylbenzene; C7HgO; J. Phys. Chem. 1993, 97, 3379-3383. [95-48-7] PREPARED BY: VARIABLES: T/K = Circa 295 (Ambient Room) W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C $x_1$ $2.9 \times 10^{-6}$ 22 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: High performance liquid chromatograph (1) Graphite soot obtained by passing an system equipped with an ultraviolet detecac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as tor aned integrator. Excess solute and solvent placed in 1-dram glass bottle and allowed to equilidetermined by mass spectrometry.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Carbon disulfide; CS <sub>2</sub> ; [75-15-0]	Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K. J. Org. Chem. 1992, 57, 6077-6079.
VARIABLES:	PREPARED BY:
T/K = 303	W.E. Acree, Jr.

# EXPERIMENTAL VALUES

phase was used.

t/°C  $c_1/(\text{mol dm}^{-3})$  $7.16 \times 10^{-3}$ 30.0

## **AUXILIARY INFORMATION**

# METHOD: APPARATUS/PROCEDURE

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

for 24 hours at ambient room temperature with agitation. Saturated solution was

filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentra-tions determined via HPLC with uv detec-

tion at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

# SOURCE AND PURITY OF MATERIALS:

 Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) Reagent grade, 99 % (or better), chem-

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

from manufacturer.

ESTIMATED ERRORS:

T/K:  $\pm$  3.

ical source not given, used as received

(2) HPLC grade or AR grade solvent, chem-ical source not given, aromatic impuri-ties removed by chromatography if necessary.

# **ESTIMATED ERRORS:**

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

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) Buckminsterfullerene; C<sub>60</sub>; Ruoff, R.S.; Tse, D.S.; Malhotra, R.; [99685-96-8] Lorents, D.C. (2) Carbon disulfide; CS2; [75-15-0] J. Phys. Chem. 1993, 97, 3379-3383. VARIABLES: PREPARED BY: T/K = Circa 295 (Ambient Room) W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C

22

6.6 x 10<sup>-4</sup>

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

## SOURCE AND PURITY OF MATERIALS:

- Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Buckminsterfullerene; C<sub>60</sub>; [99685-96-8]</li> <li>Benzonitrile; C<sub>7</sub>H<sub>5</sub>N; [100-47-0]</li> </ol>	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	<i>x</i> <sub>1</sub>
22	7.1 x 10 <sup>-5</sup>

#### AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

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

22	9.9 x 10 <sup>-5</sup>
t/°C	x <sub>1</sub>
EXPERIMENTAL VALUES	
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
variables:	PREPARED BY:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.  J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
Components:	ORIGINAL MEASUREMENTS:

#### AUXILIARY INFORMATION

## METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

## SOURCE AND PURITY OF MATERIALS:

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

- (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, Baxter Scientific Products, McGaw Park, Illinois, USA, was used as received from manufacturer.

# ESTIMATED ERRORS:

240	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Scrivens, W.A.; Tour, J.M.
(2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
22 4 x	10*4
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:
	$T/K$ : $\pm 3$ (Compiler). $c_1$ : $\pm 0.0007$ mol dm <sup>-3</sup> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ;	Scrivens, W.A.; Tour, J.M.
[99685-96-8] (2) Quinoline; C <sub>9</sub> H <sub>7</sub> N; [91-22-5]	J. Chem. Soc., Chem. Commun. 1993, 1207-1209.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
±/°C	/(mol dm <sup>-3</sup> )
22 1.0 × 10 <sup>-2</sup>	
AUXILIAR	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent sonicated and equilibrated in a room temperature bath	(2) Purity and chemical source were not
for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a	given in the paper.
0.45 $\mu$ m HPLC syringe filtered. Three	
1.0 mls were removed and placed in tared vials, which were then placed in a heated	
oil bath to facilitate solvent evaporation. Concentrations determined gravi-	

metrically from the weight of the solid

residue.

# ESTIMATED ERRORS:

r/K:  $\pm 3$  (Compiler)  $c_1$ :  $\pm 0.0007$  mol dm<sup>-3</sup>.

	24
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ;	Scrivens, W.A.; Tour, J.M.
[99685-96-8] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]	J. Chem. Soc., Chem. Commun. <u>1993</u> , 1207- 1209.
variables:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C σ₁/	$(mol dm^{-3})$
22 6 x	z 10 <sup>-4</sup>
	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Analytical balance and centrifuge.	(1) Purity and chemical source were not given in the paper.
Excess solute and solvent sonicated and equilibrated in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 $\mu$ m HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid	(2) Purity and chemical source were not given in the paper.
residue.	ESTIMATED ERRORS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C <sub>60</sub> ; [99685-96-8]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.
(2) 2-Methylthiophene; C <sub>5</sub> H <sub>6</sub> S; [554-14-3]	J. Phys. Chem. <u>1993</u> , 97, 3379-3383.
VARIABLES:	PREPARED BY:
T/K = Circa 295 (Ambient Room)	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>1</sub>	
22 9.1	x 10 <sup>-4</sup>
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.  (2) Reagent grade, 98 % (or better), chem-
filtered through a 0.45 micrometer poly- (tetrafluoroethylene) filter. Concentra- tions determined via HPLC with uv detec- tion at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary	ical source not given, used as receive from manufacturer.
toluene/hexane (20:80 by volume) mobile phase was used.	ESTIMATED ERRORS:

242

#### COMPONENTS:

- (1) Buckminsterfullerene; C<sub>60</sub>;
   [99685-96-8]
  (2) Tetrahydrothiophene; C<sub>4</sub>H<sub>8</sub>S;
- [110-01-0]

# ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. <u>1993</u>, 97, 3379-3383.

#### VARIABLES:

T/K = Circa 295 (Ambient Room)

# PREPARED BY:

W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

t/°C

22

 $3.6 \times 10^{-6}$ 

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

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

# SOURCE AND PURITY OF MATERIALS:

- Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.
- (2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

#### ESTIMATED ERRORS:

# CARBAZOLE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

### A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane

n-heptane

n-octane

n-decane

n-dodecane

n-hexadecane

cyclohexane

methylcyclohexane

cyclooctane

2,2,4-trimethylpentane

t-butylcyclohexane

squalane

decahydronaphthalene

### B. Alkenes

#### C. Aromatic Hydrocarbons

benzene

methylbenzene

1,4-dimethylbenzene

chrysene

1,2,3,4-tetrahydronaphthalene

#### D. <u>Esters</u>

ethyl ethanoate

butyl butyrate

### E. Ethers

tetrahydropyran

tetrahydrofuran

1,1-oxybisethane

1,1-oxybisbutane

1,1-oxybispentane

1,4-dioxane

methoxybenzene

### F. Haloalkanes and Haloaromatic Hydrocarbons

trichloromethane

tetrachloromethane

1-chlorohexane

1-chlorooctane

1-chlorotetradecane

chlorocyclohexane

#### G. Alcohols

methanol

ethanol

1,2-ethanediol

1-propanol
2-propanol
1-butanol
1-octanol
phenol

### H. <u>Ketones</u>

2-propanone 2-butanone cyclohexanone acetophenone

### I. Miscellaneous Pure Solvents

carbon disulfide
pyridine
quinoline
thiophene
dimethyl sulfoxide
nitromethane
acetic anhydride
1-methyl-2-pyrrolidinone
N,N-dimethylacetamide
N,N-dimethylformamide
tetramethylene sulfone
tributyl phosphate
dibenzofuran

## J. Binary Solvent Mixtures

		24			
COMPONENTS:  (1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]  (2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]  VARIABLES:		ORIGINAL MEASUREMENTS:			
		McCargar, J.W.; Acree, W.E., Jr.  Phys. Chem. Liq. 1987, 17, 123-138.  PREPARED BY:			
			T/K ≈ 298		W.E. Acree, Jr.
			EXPERIMENTAL VALUES		
t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>			
25.0	0.9999	0.000139			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature thermometer, and an ul spectrophotometer.	oath, calorimetric traviolet/visible	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.			
Excess solute and solv glass bottles and allo for several days at containment of equilibries repetitive measurement urated solutions transcoarse filter into tar flasks, weighed and di	owed to equilibrate onstant temperature. Firm verified by as aliquots of satesferred through a ged volumetric	(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.			
Concentrations determinetrically at 292 nm.	ined spectrophoto-	ESTIMATED ERRORS:			
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1.5 % (relative error).			

(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) n-Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3] VARIABLES: T/K = 298		Fung, HL.; Higuchi, T.  J. Pharm. Sci. 1987, 60, 1782-1788.  PREPARED BY:  W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
25.0	*2 0.9999	*1 0.00017	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROC Constant temperature thermometer, and an uspectrophotometer. Excess solute and sol glass bottles and all for 24 hours at const Attainment of equilib repetitive measurement urated solutions transcoarse filter into ta flasks, weighed and of	bath, calorimetric altraviolet/visible  event placed in amber and temperature.  orium verified by the aliquots of sature afterned through a seried volumetric	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.  (2) ACS Reagent Grade, source not specified, was used as received.	
Concentrations determined spectrophoto- metrically at 292.5 nm.		ESTIMATED ERRORS: $T/K$ : $\pm$ 0.1 (compiler). $x_1$ : $\pm$ 3 % (relative error, compiler).	

ORIGINAL MEASUREMENTS:

240			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]		McCargar, J.W.; Acree, W.E., Jr.  Phys. Chem. Liq. <u>1987</u> , 17, 123-138.	
			VARIABLES:
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	
25.0	0.9998	0.000173	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature thermometer, and an ul spectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.	
Excess solute and solve glass bottles and allo for several days at containment of equilibrate repetitive measurement urated solutions transcoarse filter into tar flasks, weighed and di	wed to equilibrate onstant temperature. it is verified by s. Aliquots of sat-iferred through a red volumetric luted with methanol.	(2) HPLC Grade, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.	
Concentrations determine metrically at 292 nm.	.ned spectrophoto-	ESTIMATED ERRORS:	
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1.5 % (relative error).	

(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]		ORIGINAL MEASUREMENTS:	
		Fung, HL.; Higuchi, T.  J. Pharm. Sci. 1987, 60, 1782-1788.	
			VARIABLES:
T/K = 298		W.E. Acree, Jr.	
EIPERIMENTAL VALUES			
t/°C	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	
25.0	0.9998	0.00023	

#### **AUXILIARY INFORMATION**

#### METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
- (2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.

# ESTIMATED ERRORS:

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

		Δ4:			
COMPONENTS:  (1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]  (2) n-Octane; C <sub>8</sub> H <sub>18</sub> ; [111-65-9]  VARIABLES:		ORIGINAL MEASUREMENTS:			
		McCargar, J.W.; Acree, W.E., Jr.  Phys. Chem. Liq. 1987, 17, 123-138.  PREPARED BY:			
			T/K = 298		W.E. Acree, Jr.
			EXPERIMENTAL VALUES		
t/°C	<b>*</b> 2	x <sub>1</sub>			
25.0	0.9998	0.000198			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCI	EDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature in thermometer, and an unspectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.			
Excess solute and solute glass bottles and alle for several days at containment of equilibries transcoarse filter into tai flasks, weighed and different solutions.	owed to equilibrate onstant temperature. rium verified by ts. Aliquots of satsered through a red volumetric	(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.			
Concentrations determinetrically at 292 nm.	ined spectrophoto-	ESTIMATED ERRORS:			
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1.5 % (relative error).			

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

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

spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by

repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetrachloromethane. Concentrations determined

spectrophotmetrically at 292 nm.

248			
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) n-Dodecane; C <sub>12</sub> H <sub>26</sub> ; [112-40-3]		ORIGINAL MEASUREMENTS:	
		Fung, HL.; Higuchi, T.	
		J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.	
VARIABLES:		PREPARED BY:	
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	<b>x</b> <sub>2</sub>	× <sub>1</sub>	
25.0	0.9997	0.00032	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCED	URE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature ba thermometer, and an ult spectrophotometer.		(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.	
Excess solute and solver glass bottles and allow for 24 hours at constant Attainment of equilibric repetitive measurements urated solutions transf coarse filter into tare flasks, weighed and dil	ed to equilibrate t temperature. um verified by . Aliquots of sat- erred through a d volumetric	(2) Reagent Grade, source not specified, was passed through a silica gel column.	
Concentrations determine metrically at 292.5 nm.	ed spectrophoto-	ESTIMATED ERRORS:	
		$T/K$ : $\pm$ 0.1 (compiler). $x_1$ : $\pm$ 3 % (relative error, compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) n-Hexadecane; C <sub>16</sub> H <sub>34</sub> ; [544-76-	J. Pharm. Sci. <u>1987</u> , 76, 572-574.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	x <sub>1</sub>
25.0 0.999	0.000414
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calori thermometer, and an ultraviolet/v	

# ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_1$ :  $\pm$  2 % (relative error).

lized 3 times from absolute ethanol.

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

	2
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Fung, HL.; Higuchi, T.  J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.
(2) n-Hexadecane; C <sub>16</sub> H <sub>34</sub> ; [544-76-3]	
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	× <sub>1</sub>
25.0 0.9996	0.00059
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1 (compiler). $x_1$ : $\pm$ 3 % (relative error, compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	<b>x</b> 1
25.0 0.9998	0.000183
AUXILIA	LRY 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	Company, was stored over molecular sieves and distilled shortly before use
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>10</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.  Collection Czech. Chem. Commun. 1967, 32, 931-943.  PREPARED BY:
(2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]	
VARIABLES:	
T/K = 293 and 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C × <sub>2</sub>	x <sub>1</sub>
20.0 0.999+	0.000153
25.0 0.999+	0.000224
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.  (2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.05. $x_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Fung, HL.; Higuchi, T.
(2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-	J. Pharm. Sci. <u>1987</u> , 60, 1782-1788.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>
25.0 0.9	998 0.00018
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calc thermometer, and an ultraviolet spectrophotometer.	
Excess solute and solvent place glass bottles and allowed to experience and allowed to experience attainment of equilibrium verification repetitive measurements. Alique urated solutions transferred to coarse filter into tared volume flasks, weighed and diluted with	was distilled over phosphorous pent- ature. oxide. ied by ts of sat- rough a tric
Concentrations determined spect metrically at 292.5 nm.	rophoto- ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1 (compiler). $x_1$ : $\pm$ 3 % (relative error, compiler).

		25			
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]		ORIGINAL MEASUREMENTS:			
		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>			
320.6	0.9993	0.00066			
321.1	0.9992	0.00083			
325.1	0.9989	0.00106			
357.2	0.9971	0.00293			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCED	URE	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		<ul> <li>(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.</li> <li>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</li> </ul>			
noting the temperature at which the last trace of solid solute disappeared.		ESTIMATED ERRORS:			
Julio di Solla Bollada a	anabbanean,	T/K: precision ± 0.1. x <sub>1</sub> : ± 0.0003.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-	-8] McCargar, J.W.; Acree, W.E., Jr.
(2) Methylcyclohexane; C <sub>7</sub> H <sub>14</sub> ; [108-87-2]	Phys. Chem. Liq. 1987, 17, 123-138.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	× <sub>2</sub> × <sub>1</sub>
25.0	0.000196
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, cathermometer, and an ultraviol spectrophotometer.	
Excess solute and solvent plaglass bottles and allowed to for several days at constant Attainment of equilibrium ver repetitive measurements. Aliquiated solutions transferred coarse filter into tared voluflasks, weighed and diluted w	equilibrate temperature. rified by quots of sat- through a metric with methanol.  Chemical Company, was stored over molecular sieves and distilled shortly before use.
Concentrations determined spe metrically at 292 nm.	
	$T/K$ : $\pm 0.05$ . $x_i$ : $\pm 1.5$ % (relative error).

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Cyclooctane; C <sub>8</sub> H <sub>16</sub> ; [292-64-8]  VARIABLES:		McCargar, J.W.; Acree, W.E., Jr.			
		Phys. Chem. Liq. 1987, 17, 123-138.  PREPARED BY:			
					T/K = 298
EIPERIMENTAL VALUES					
t/°C	×2	x <sub>1</sub>			
25.0	0.9997	0.000309			
	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 292 nm.	ned spectrophoto-	ESTIMATED ERRORS:			
		T/K: ± 0.05. x,: ± 1.5 % (relative error).			

COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.				
(2) 2,2,4-Trimethylpentane; C <sub>8</sub> H <sub>18</sub> ; [540-84-1]	Phys. Chem. Liq. <u>1987</u> , 17, 123-138.				
VARIABLES:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EIPERIMENTAL VALUES					
t/°C ≭₂	×1				
25.0 0.9999	0.000126				
AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.				
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.				
Concentrations determined spectrophoto- metrically at 292 nm.	ESTIMATED ERRORS:				
	$T/K: \pm 0.05.$ $x_1: \pm 1.5 $ % (relative error).				

	25			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Fung, HL.; Higuchi, T.			
(2) 2,2,4-Trimethylpentane; C <sub>8</sub> H <sub>18</sub> ; [540-84-1]	J. Pharm. Sci. 1987, 60, 1782-1788.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>			
25.0 0.9998	0.00018			
METHOD: APPARATUS/PROCEDURE  Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	SOURCE AND PURITY OF MATERIALS:  (1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was distilled over sodium.			
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:			
	$T/K$ : $\pm$ 0.1 (compiler). $x_1$ : $\pm$ 3 % (relative error, compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.  Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).				
(2) 2,2,4-Trimethylpentane; C <sub>8</sub> H <sub>18</sub> ; [540-84-1]					
variables:	PREPARED BY:				
T/K = 298	W.E. Acree, Jr.				
EXPERIMENTAL VALUES					
t/°C ¢ <sub>1</sub> ,	/(mol dm <sup>-3</sup> )				
25.0 0.00077					
	Y INFORMATION				
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
	1				
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.				
thermometer, and an ultraviolet/visible	waukee, Wisconsin, USA, was recrystal-				

T/K:  $\pm$  0.1 (compiler).  $c_1$ :  $\pm$  3 % (relative error; compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]		McCargar, J.W.; Acree, W.E., Jr.				
(2) t-Butylcyclohexand [3178-22-1]	e; C <sub>10</sub> H <sub>20</sub> ;	J. Solution Chem. <u>1988</u> , 17, 1081-1091.				
VARIABLES:		PREPARED BY:				
T/K = 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°C	<b>x</b> <sub>2</sub>	× <sub>1</sub>				
25.0	0.9997	0.000250				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature in thermometer, and an unspectrophotometer.		(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.				
Excess solute and solutions bottles and alle for several days at containment of equilibrated solutions transcoarse filter into tar flasks, weighed and di	owed to equilibrate onstant temperature. rium verified by the Aliquots of satesferred through a red volumetric	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and dis- tilled shortly before use.				
Concentrations determine metrically at 292 nm.	ined spectrophoto-	ESTIMATED ERRORS:				
		$T/K: \pm 0.05.$ $x_1: \pm 1.5 \%$ (relative error).				

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	McCargar, J.W.; Acree, W.E., Jr.			
(2) 2,6,10,15,19,23-Hexamethyltetraco- sane (squalane); C <sub>30</sub> H <sub>62</sub> ; [111-01-3]	J. Pharm. Sci. <u>1987</u> , 76, 572-574.			
VARIABLES:	PREPARED BY:			
T/K = 298	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C × <sub>2</sub>	<del>x</del> 1			
25.0 0.9993	0.000671			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.			
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetra-	(2) 99 %, Aldrich Chemical Company, was used as received.			
chloromethane. Concentrations determined spectrophotmetrically at 292 nm.	ESTIMATED ERRORS:			
	$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 2 % (relative error).			

(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Decahydronaphthalene; C <sub>10</sub> H <sub>18</sub> ; [91-17-8]		ORIGINAL MEASUREMENTS:  Coon, J.E.; Auwaerter, J.E.; McLaughlin,			
		VARIABLES:		PREPARED BY:	
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>			
333.3	0.9974	0.00263			
348.7	0.9959	0.00414			
357.6	0.9946	0.00544			
361.6	0.9944	0.00557			
376.0	0.9890	0.01098			
388.2	0.9812	0.01880			
402.2	0.9719	0.02811			
416.2	0.9503	0.04967			
438.2	0.9047	0.09527			
473.2	0.7009	0.29909			
491.7	0.4945	0.50551			
502.2	0.3085	0.69153			

#### AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
- (2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

#### ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Carbazole; C <sub>12</sub> H <sub>10</sub> N; [86-74-8] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]		Smutek, M.; Fris, M.; Fohl, J.				
		Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.				
VARIABLES:		PREPARED BY:				
T/K = 293 and 298		W.E. Acree, Jr.				
EXPERIMENTAL VALUES						
t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>				
20.0	0.996	0.00352				
25.0	0.996	0.00412				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEDU	JRE	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		<ul> <li>(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.</li> <li>(2) 99 %, Commercial sample, source and purification method was not specified.</li> </ul>				
weight of solid residue after solvent had evapor	that remained	ESTIMATED ERRORS:  T/K: precision ± 0.05.  x <sub>1</sub> : ± 3 % (relative error; compiler).				

COMPONENTS:  (1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]  (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]  VARIABLES:  Temperature		ORIGINAL MEASUREMENTS:  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 V	VALUES		
T/K	* <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	× <sub>1</sub>
307.1	0.9946	0.0054	326.8	0.9891	0.0109
310.3	0.9932	0.0068	340.3	0.9866	0.0134
313.2	0.9937	0.0063			
324.1	0.9907	0.0093			
		AUXILIARY	INFORMATION	ſ	
METHOD: APPARI	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:
Constant temperature bath and a precision thermometer.			Wisconsin, U	mical Company, Milwau- SA, was used as	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.			
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.		T/K: prec x <sub>1</sub> : ± 0.0	ision ± 0.1.		

						20
COMPONENTS:  (1) Carbazole; C <sub>12</sub> H <sub>10</sub> N; [86-74-8]  (2) Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]  VARIABLES:  T/K = 293, 313 and 333		ORIGINAL MEASUREMENTS: Smutek, M.; Fris, M.; Fohl, J.				
						Collection Czech. Chem. Commun. 1967, 32, 931-943.
		PREPARED BY:				
		W.E. Acree, Jr.				
		EXPERIMENTAL	VALUES			
t/°C	×2	<i>x</i> <sub>1</sub>	t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	
20.0	0.996	0.00374	60.0	0.989	0.0111	
40.0	0.993	0.00666				
***************************************		AUXILIARY	INFORMATIO	N		
METHOD: APPAR	ATUS/PROCEDU	RE	SOURCE AN	D PURITY OF	MATERIALS:	
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from		<ul> <li>(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.</li> <li>(2) 99 %, Commercial sample, source and purification method was not specified.</li> </ul>			ive and	
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) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) 1,4-Dimethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [106-42-3]  VARIABLES:  T/K = 293		ORIGINAL MEASUREMENTS:		
		Smutek, M.; Fris, M.; Fohl, J.  Collection Czech. Chem. Commun. 1967, 32, 931-943.  PREPARED BY:		
			W.E. Acree, Jr.	
			EXPERIMENTAL VALUES	
		t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>
20.0 0.995		0.00483		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:		
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed class container and allowed to equilibrate		(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.		

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

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

ESTIMATED ERRORS:

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.

COMPONENTS:  (1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]  (2) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [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	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>
				528.2	1.000	0.000
				519.7	0.903	0.097
511.2	0.805	0.195				
500.7	0.698	0.302				
493.4	0.606	0.394				
482.9	0.505	0.495				
478.4	0.472	0.528				
477.2	0.445	0.555				
479.8	0.396	0.604				
484.7	0.347	0.653				
489.6	0.301	0.699				
499.2	0.200	0.800				
507.5	0.108	0.892				
517.2	0.000	1.000				
	AUXILIARY	INFORMATION				
METHOD: APPARATUS/PROCEI	DURE	SOURCE AND PURITY OF MATERIALS:				
Phase diagram was deter thermal analysis method detail in V.M. Kravcher U.S.S.R. 1939, 13, 133 visual observations.	d (described in nko, J. Phys. Chem.	(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:  (1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]  (2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2]  VARIABLES:  Temperature			ORIGINAL M	EASUREMENTS:					
		Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.							
		Fluid Phase Equilibr. 1989, 44, 305-345.  PREPARED BY:  W.E. Acree, Jr.							
				EXPERIMENTAL V	ALUES				
				T/K	<i>x</i> <sub>2</sub>	<i>×</i> <sub>1</sub>	T/K	x <sub>2</sub>	x <sub>1</sub>
344.7	0.9927	0.0073	495.2	0.3029	0.6971				
374.8	0.9897	0.0103							
476.2	0.7113	0.2887							
		AUXILIARY	INFORMATION	ī					
METHOD: APPARATUS/PROCEDURE		SOURCE AND	PURITY OF M	ATERIALS:					
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			e, Wisconsin	emical Company, Mil- , USA, was used as					
		store		Chemical Company, was ular sieves to remove					
noting the te	emperature at	which the last	ESTIMATED	ERRORS:					
trace of solid solute disappeared.		T/K: prec x <sub>1</sub> : ± 0.00	ision ± 0.1.						

Components:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
(2) Ethyl ethanoate; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ; [141-78-6]		
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
* <sub>2</sub>		
0.980 0.0	20	
AUXILIARY	INFORMATION	
	INFORMATION SOURCE AND PURITY OF MATERIALS:	
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.
(2) Butyl butyrate; C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [109-21-7]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.

#### EXPERIMENTAL VALUES

 $t/^{\circ}C$   $c_1/(\text{mol dm}^{-3})$  25.0 0.0994

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.
- (2) Purity not given, Eastman Chemical Co., Rochester, New York, USA, was shaken with sodium hydroxide, washed with distilled water, dried over magnesium sulfate and distilled. Stored over molecular sieves and distilled shortly before use.

#### ESTIMATED ERRORS:

T/K:  $\pm$  0.1 (compiler).  $c_1$ :  $\pm$  3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Carbazole; C<sub>12</sub>H<sub>9</sub>N; [86-74-8]</li> <li>(2) Tetrahydropyran; C<sub>5</sub>H<sub>10</sub>O; [142-68-7]</li> </ul>	Acree, W.E., Jr.; McCargar, J.W.; Zvaigzne, A.I.; Teng, IL. Phys. Chem. Liq. 1991, 23, 27-35.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.

#### AUXILIARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

# SOURCE AND PURITY OF MATERIALS:

- (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.
- (2) 99 %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

#### ESTIMATED ERRORS:

T/K:  $\pm$  0.05.  $x_1$ :  $\pm$  4 % (relative error).

# ORIGINAL MEASUREMENTS: COMPONENTS: Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation) (1) Carbazole; C<sub>12</sub>H<sub>0</sub>N; [86-74-8] (2) Tetrahydrofuran; C4HgO; [109-99-9] PREPARED BY: VARIABLES: W.E. Acree, Jr. T/K = See below EXPERIMENTAL VALUES $x_2$ *x*<sub>1</sub> 0.929 0.071 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: (1) Purity and chemical source not specified in paper. No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which indepen-dently determined values exist, compiler estimates the temperature as between 298-303 K. (2) Purity and chemical source not specified in paper. ESTIMATED ERRORS:

T/K: Unknown.

ORIGINAL MEASUREMENTS:

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

(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) 1,1-Oxybisethane; C <sub>4</sub> H <sub>10</sub> O; [60-29-7]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub> x <sub>1</sub>		
0.987 0.0	13	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
the paper.	fied in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).	

202		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Fung, HL.; Higuchi, T.	
(2) 1,1-Oxybisethane; C <sub>4</sub> H <sub>10</sub> O; [60-29-7]	J. Pharm. Sci. 1987, 60, 1782-1788.  PREPARED BY:	
variables:		
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	$x_1$	
25.0 0.9870	0.0130	
AUXILIAR	Y INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.	(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.	
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether.	(2) Reagent Grade, source not specified, was distilled from lithium aluminum hydride shortly before use.	
Concentrations determined spectrophoto- metrically at 292.5 nm.	ESTIMATED ERRORS:	
	$T/K$ : $\pm$ 0.1 (compiler). $x_1$ : $\pm$ 3 % (relative error, compiler).	

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

coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

# ESTIMATED ERRORS:

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

	200	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.	
(2) 1,1 -Oxybisbutane; C <sub>8</sub> H <sub>18</sub> O; [142-96-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
VARIABLES:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C	(mol dm <sup>-3</sup> )	
25.0 0.03	287	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99 %, Aldrich Chemical Company, was used as received.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	T/K: ± 0.1 (compiler). c.: + 3 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.  Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).	
(2) 1,1 -Oxybispentane; C <sub>10</sub> H <sub>22</sub> O; [693-65-2]		
variables:	PREPARED BY:	
T/K = 298	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
t/°C		
25.0 0.0	0182	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
AUXILIARY	INFORMATION	
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.	
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Purity not given, Pfaltz and Bauer, Waterbury, Connecticut, USA, was treated with potassium permanganate, washed with distilled water and sulfuric acid solution, dried over calcium chloride and distilled before use.	
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:	
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
(2) 1,4-Dioxane; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ; [123-91-1]		
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub> x <sub>1</sub>		
0.964 0.0	036	
AUXILIARY	( INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	<ol> <li>Purity and chemical source not speci- fied in paper.</li> </ol>	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).	

<ul> <li>(1) Carbazole; C<sub>12</sub>H<sub>9</sub>N; [86-74-8]</li> <li>(2) Methoxybenzene; C<sub>7</sub>H<sub>8</sub>O; [100-66-3]</li> </ul>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x <sub>2</sub> x <sub>1</sub>	
0.987 0.0	013
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:

ORIGINAL MEASUREMENTS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	Collection Czech. Chem. Commun. 1967, 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	$x_1$
25.0 0.9	0.00478
	AUXILIARY INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, there and a precision balance.  Excess solute and solvent places glass container and allowed to for several hours at constant to Aliquots of saturated solutions transferred into tared constainweighed. Solubilities calculate	several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.  equilibrate emperature.  (2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that resafter solvent had evaporated.	

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N;	[86-74-8]	Fung, HL.; Higuchi, T.
(2) Trichloromethane; [67-66-3]	CHCl <sub>3</sub> ;	J. Pharm. Sci. 1987, 60, 1782-1788.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EIPERIMENTAL VALUES		
t/°C	× <sub>2</sub>	<b>x</b> <sub>1</sub>
25.0	0.9963	0.0037
		and the second s
	AUXIL	IARY INFORMATION

#### METHOD: APPARATUS/PROCEDURE

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

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

# SOURCE AND PURITY OF MATERIALS:

- Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.
- (2) Reagent Grade, source not specified, was washed with distilled water five times, stored overnight over calcium chloride and distilled from phosphorous pentoxide.

#### ESTIMATED ERRORS:

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

266	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.
(2) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
25.0 0.0	468
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) Purity not given, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was washed with distilled water, stored over calcium chloride and distilled shortly before use.
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:

COMPONENTS:			ORIGINAL	MEASUREMENTS	•
(1) Carbazol	.e; C <sub>12</sub> H <sub>9</sub> N; [8	6-74-8]	Smutek,	M.; Fris, M.	; Fohl, J.
(2) Tetraclo [56-23-5	romethane; C	Cl <sub>4</sub> ;	Collecti 32, 931-		em. Commun. <u>1967</u> ,
VARIABLES:			PREPARED	BY:	
T/K = 293, 2	98, 313 and	333	W.E. Acr	ee, Jr.	
		333	W.E. Acr	ree, Jr.	
		333 *1	w.E. Acr	x <sub>2</sub>	×1
EXPERIMENTAL	VALUES				× <sub>1</sub> 0.00165

# AUXILIARY INFORMATION

# METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

# SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

T/K:  $\pm$  0.1 (compiler).  $c_1$ :  $\pm$  3 % (relative error; compiler).

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

# ESTIMATED ERRORS:

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

COMPONENTS:	<del></del>	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N;	[86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) 1-Chlorohexane; C <sub>6</sub> H [544-10-5]	i <sub>13</sub> C1;	J. Solution Chem. <u>1989</u> , 18, 151-158.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	<b>x</b> <sub>2</sub>	$x_1$
25.0	0.9974	0.00255
<u> </u>	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature be thermometer, and an ule 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 conditional and attainment of equilibrate repetitive measurements urated solutions transcoarse filter into tarflasks, weighed and di	wed to equilibrate nstant temperature. ium verified by s. Aliquots of sat- ferred through a ed volumetric	(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.
Concentrations determine metrically at 292 nm.		ESTIMATED ERRORS:
		$T/K$ : $\pm 0.05$ . $x_1$ : $\pm 1.5$ % (relative error).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N;	[86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) 1-Chlorooctane; C <sub>8</sub> [111-85-3]	H <sub>17</sub> Cl;	J. Solution Chem. 1989, 18, 151-158.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	<b>*</b> 2	x <sub>1</sub>
25.0	0.9976	0.00242
	AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature be thermometer, and an ule spectrophotometer.  Excess solute and solve glass bottles and allowed for several days at containment of equilibrians.	ent placed in amber wed to equilibrate nstant temperature.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal- lized 3 times from absolute ethanol.  (2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly
repetitive measurement urated solutions trans coarse filter into tar flasks, weighed and di	s. Aliquots of sat- ferred through a ed volumetric luted with methanol.	before use.
Concentrations determine metrically at 292 nm.	ned spectrophoto-	ESTIMATED ERRORS:
		$T/K$ : $\pm$ 0.05. $x_1$ : $\pm$ 1.5 % (relative error).

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Carbazole; C<sub>12</sub>H<sub>0</sub>N; [86-74-8] McCargar, J.W.; Acree, W.E., Jr. (2) 1-Chlorotetradecane; C16H20Cl; J. Solution Chem. 1989, 18, 151-158. [2425-54-9] PREPARED BY: VARIABLES: T/K = 298W.E. Acree, Jr. EXPERIMENTAL VALUES t/°C  $x_2$ 0.9976 0.00240 25.0 AUXILIARY INFORMATION METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystal-lized 3 times from absolute ethanol. Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of sat-Aldrich Chemical Company, was (2) 99 %, treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use. urated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm. ESTIMATED ERRORS:  $T/K: \pm 0.05.$  $x_1$ :  $\pm 1.5$  % (relative error).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N;	[86-74-8]	McCargar, J.W.; Acree, W.E., Jr.
(2) Chlorocyclohexane [542-18-7]	; C <sub>6</sub> H <sub>11</sub> Cl;	J. Solution Chem. <u>1989</u> , 18, 151-158.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	* <sub>2</sub>	<b>x</b> <sub>1</sub>
25.0	0.9971	0.00291
	AUXIL	IARY INFORMATION
METHOD: APPARATUS/PROC	EDURE	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 292 nm.

- (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.
- (2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.

### **ESTIMATED ERRORS:**

 $x_1$ :  $\pm$  1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) Methanol; CH <sub>4</sub> O; [67-56-1]	Collection Czech. Chem. Commun. 1967, 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C ×2	x <sub>1</sub>
20.0 0.998	0.00183
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.  (2) 99 %, Commercial sample, source and purification method was not specified.
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:
	$T/K$ : precision $\pm$ 0.05. $x_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) Ethanol; C <sub>2</sub> H <sub>6</sub> O; [64-17-5]	Collection Czech. Chem. Commun. <u>1967</u> , 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C × <sub>2</sub>	x <sub>1</sub>
20.0 0.997	0.00332
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	<ol> <li>(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.</li> <li>(2) 99 %, Commercial sample, source and purification method was not specified.</li> </ol>
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N,	; [86 <del>-</del> 74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.	
(2) Ethanol; C <sub>2</sub> H <sub>6</sub> O; [	64-17-5]	Int. J. Pharm. 1994, 104, 125-133.	
ARIABLES:		PREPARED BY:	
T/K = 298		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
t/°C	×2	<b>x</b> <sub>1</sub>	
25.0	0.9964	0.00358	
ETHOD: APPARATUS/PROC	CEDURE	SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROC	CEDURE	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not given	
and an ultraviolet/vimeter.	sible spectrophoto-	in paper.	
Excess solute and sol glass bottles and all at constant temperate determined spectropho 292 nm.	lowed to equilibrate are. Concentrations	(2) Purity and chemical source not given in paper.	
		ESTIMATED ERRORS:	
		$T/K$ : $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 3 % (relative error, Compiler).	
		I	

(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Ethanol; C <sub>2</sub> H <sub>6</sub> O; [64-17-5]  VARIABLES:	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)  PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
ж <sub>2</sub> ж <sub>1</sub>	
0.9886 0.0	114
AUXILIARY	INFORMATION
	INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-

ORIGINAL MEASUREMENTS:

	<b>-</b> '
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) 1,2-Ethanediol; C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> ; [107-21-1]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1985, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K ≈ See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x <sub>2</sub>	
0.993 0.0	07
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.
(2) 1-Propanol; C <sub>3</sub> H <sub>8</sub> O; [71-23-8]	Int. J. Pharm. <u>1994</u> , 104, 125-133.
variables:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	<b>x</b> 1
25.0 0.9963	0.00365
AUXILIAN	Y INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and an ultraviolet/visible spectrophotometer.	(1) Purity and chemical source not given in paper.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.	(2) Purity and chemical source not given in paper.
	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 3 % (relative error, Compiler).

COMPONENTS:			ORIGINAL 1	MEASUREMENTS:	•
(1) Carbazol	e; C <sub>12</sub> H <sub>9</sub> N; [8	6-74-8]	Smutek, 1	M.; Fris, M.;	; Fohl, J.
(2) 2-Propan	nol; C <sub>3</sub> H <sub>8</sub> O; [6	7-63-0]	Collection 32, 931-		em. Commun. <u>1967</u> ,
VARIABLES:			PREPARED	BY:	
T/K = 293, 3	313 and 333		W.E. Acr	ee, Jr.	
EXPERIMENTAL	VALUES				
t/°C	<b>x</b> 2	<i>x</i> <sub>1</sub>	t/°C	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>
20.0	0.997	0.00277	60.0	0.991	0.00912
40.0	0.995	0.00523			
		AUXILIARY	INFORMATIO	N	
METHOD: APPAR	RATUS/PROCEDU	RE	SOURCE AND	D PURITY OF 1	MATERIALS:
Excess solut glass contai for several Aliquots of transferred weighed. So	ion balance.  e and solvent iner and allow hours at cons saturated sol into tared co- blubilities ca-	onstainers and alculated from	seve: pyric a fin	ral times fro dine, and the nal purity of , Commercial	, was recrystallized om toluene and en sublimed to give f 98.3 %. sample, source and nod was not specified
	olid residue t at had evapora		ESTIMATED	ERRORS:	•
					error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.
(2) 1-Butanol; C <sub>4</sub> H <sub>10</sub> O; [71-36-3]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
variablës:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
25.0 0.0	493
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) puriss, 99.5 %, Fluka Chemical Corpora- tion, Ronkonkoma, New York, USA, was stored over molecular sieves to remove trace water.
Concentrations determined spectrophotometrically at 356 nm.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).

Components:		ORIGINAL MEASUREMENTS:
(1) Carbazole; (	: <sub>12</sub> H <sub>9</sub> N; [86~74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.
(2) 1-Butanol; (	<sup>2</sup> 4H <sub>10</sub> O; [71-36-3]	Int. J. Pharm. 1994, 104, 125-133.
VARIABLES:		PREPARED BY:
T/K = 298		W.E. Acree, Jr.
EXPERIMENTAL VALU	ES	
t/°C	*2	<b>x</b> <sub>1</sub>
25.0	0.9956	0.00444
ETHOD: APPARATUS		SOURCE AND PURITY OF MATERIALS:
Constant tempera	ture bath, thermometer, et/visible spectrophoto-	(1) Purity and chemical source not given in paper.
glass bottles an at constant temp	d solvent placed in amber d allowed to equilibrate erature. Concentrations rophotometrically at	(2) Purity and chemical source not given in paper.
		ESTIMATED ERRORS:  T/K: ± 0.2 (Compiler).  x,: ± 3 % (relative error, Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Anderson, B.D.
(2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [540-84-1]	Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	PREPARED BY:
T/K ≈ 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
25.0 0.0	515
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
	INFORMATION
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.	(1) 99+ %, Aldrich Chemical Company, Mil- waukee, Wisconsin, USA, was recrystal- lized from acetone-heptane mixtures.
•	<u> </u>
Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol.	(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.
Concentrations determined spectrophoto- metrically at 356 nm.	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).

274	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Ruelle, P.; Sarraf, E.; Kesselring, U.W.
(2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [540-84-1]	Int. J. Pharm. <u>1994</u> , 104, 125-133.
VARIABLES:	PREPARED BY:
T/K # 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	$\mathbf{x_{t}}$
25.0 0.9919	0.00806
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, thermometer, and an ultraviolet/visible spectrophotometer.	(1) Purity and chemical source not given in paper.
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.	(2) Purity and chemical source not given in paper.
	ESTIMATED ERRORS:
	$T/K$ : $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 3 % (relative error, Compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N;	[86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) Phenol; C <sub>6</sub> H <sub>6</sub> O; [108	-95-2]	Collection Czech. Chem. Commun. 1967, 32, 931-943.
VARIABLES:		PREPARED BY:
T/K = 313		W.E. Acree, Jr.
EXPERIMENTAL VALUES		
t/°C	* <sub>2</sub>	<b>x</b> <sub>1</sub>
40.0	0.994	0.00598
	AUXIL	IARY INFORMATION

### METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.
- (2) 99 %, Commercial sample, source and purification method was not specified.

#### ESTIMATED ERRORS:

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

	21
Components:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.
(2) 2-Propanone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1]	Collection Czech. Chem. Commun. 1967, 32, 931-943.
VARIABLES:	PREPARED BY:
T/K = 293	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C x <sub>2</sub>	<i>x</i> <sub>1</sub>
20.0 0.976	0.0239
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	<ul> <li>(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.</li> <li>(2) 99 %, Commercial sample, source and purification method was not specified.</li> </ul>
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).

(2) 2-Propanone; C	H <sub>9</sub> N; [86-74-8] ; <sub>3</sub> H <sub>6</sub> O; [67-64-1]		Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:			PREPARED BY:
T/K = See below			W.E. Acree, Jr.
EXPERIMENTAL VALUES			
	<b>x</b> 2	×1	
	0.9628	0.03	372
METHOD: APPARATUS/P	ROCEDURE		SOURCE AND PURITY OF MATERIALS:
METHOD: APPARATUS/P	ROCEDURE		SOURCE AND PURITY OF MATERIALS:
No experimental de	tails were given	in	(1) Purity and chemical source not speci-
No experimental de the paper.	tails were given	in	(1) Purity and chemical source not speci- fied in paper.
	ental values givents for which is values exist, con	en in ndepen- mpiler	
the paper.  Based upon experim the paper for solv dently determined estimates the temp	ental values givents for which is values exist, con	en in ndepen- mpiler	fied in paper.  (2) Purity and chemical source not speci-

ORIGINAL MEASUREMENTS:

.76	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) 2-Butanone; C <sub>2</sub> H <sub>8</sub> O; [78-93-3]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44.
(2) 2 2000.000, 04.180, (10 10 0)	(English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
* <sub>2</sub>	
0.9576 0.0	424
AUXILIARY	INFORMATION
METROD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	T/K: Unknown.
	$x_1$ : $\pm$ 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) Cyclohexanone; C <sub>6</sub> H <sub>10</sub> O; [108-94-1]	V.V.; Nazarov, V.N.; Vail, E.I.  Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
variables:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
$x_2$ $x_1$	
0.932 0.00	58
	INFORMATION
AUXILIARY METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.	INFORMATION  SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-
No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	<ul><li>SOURCE AND PURITY OF MATERIALS:</li><li>(1) Purity and chemical source not specified in paper.</li><li>(2) Purity and chemical source not speci-</li></ul>

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)		
(2) Acetophenone; C <sub>8</sub> H <sub>8</sub> O; [98-86-2]			
VARIABLES:	PREPARED BY:		
T/K = See below	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
$x_2$ $x_1$			
0.959 0.0	0.041		
	INFORMATION		
ETHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.		
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.		
	ESTIMATED ERRORS:		
	T/K: Unknown. x,: ± 8 % (relative error; compiler).		

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.			
(2) Carbon disulfide; CS <sub>2</sub> ; [75-15-0]	Collection Czech. Chem. Commun. 1967, 32, 931-943.			
VARIABLES:	PREPARED BY:			
T/K = 293	W.E. Acree, Jr.			
EXPERIMENTAL VALUES				
t/°C x <sub>2</sub>	<b>×</b> 1			
20.0 0.999	0.00149			
AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	<ul> <li>(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.</li> <li>(2) 99 %, Commercial sample, source and purification method was not specified.</li> </ul>			
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:  T/K: precision ± 0.05.  x <sub>1</sub> : ± 3 % (relative error; compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Smutek, M.; Fris, M.; Fohl, J.				
(2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]	Collection Czech. Chem. Commun. 1967, 32, 931-943.  PREPARED BY:				
VARIABLES:					
T/K = 293, 313 and 333	W.E. Acree, Jr.				
EXPERIMENTAL VALUES					
t/°C	$t/^{\circ}C$ $x_2$ $x_1$				
20.0 0.911 0.0895	60.0 0.862 0.138				
40.0 0.890 0.110					
AUXILIARY INFORMATION					
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:				
Constant temperature bath, thermometer, and a precision balance.  Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from	(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.  (2) 99 %, Commercial sample, source and purification method was not specified.				
weight of solid residue that remained after solvent had evaporated.	ESTIMATED ERRORS:				
	$T/K$ : precision $\pm$ 0.05. $x_1$ : $\pm$ 3 % (relative error; compiler).				

COMPONENTS:			ORIGINAL ME	ORIGINAL MEASUREMENTS:  Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.		
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]		McLaughlin				
VARIABLES:			PREPARED BY	PREPARED BY:		
Temperature		W.E. Acree	, Jr.			
EXPERIMENTAL	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	× <sub>2</sub>	$x_1$	
301.5	0.9023	0.0977	400.7	0.7376	0.2624	
318.1	0.8852	0.1148	439.2	0.6167	0.3833	
345.5	0.8510	0.1490				
370.3	0.8041	0.1959				

AUXILIARY INFORMATION

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

#### SOURCE AND PURITY OF MATERIALS:

- (1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
- (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

#### ESTIMATED ERRORS:

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

	27
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,
(2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	<del> </del>
x <sub>2</sub> x <sub>1</sub>	
0.914 0.086	
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. x <sub>1</sub> : ± 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Quinoline; C <sub>9</sub> H <sub>7</sub> N; [91-22-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x <sub>2</sub>	
0.879 0.1	21
	INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.
the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	(2) Purity and chemical source not specified in paper.
303 к.	
303 к.	ESTIMATED ERRORS:

<u>,</u>			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	
313.7	0.9893	0.0107	
337.1	0.9796	0.0204	
345.6	0.9746	0.0254	
349.5	0.9713	0.0287 .	
	AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEI	DURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bathermometer.	-	<ol> <li>99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was used as received.</li> </ol>	
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.	
noting the temperature	at which the last	ESTIMATED ERRORS:	
trace of solid solute of	isappeared.	$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Dimethylsulfoxide; C <sub>2</sub> H <sub>6</sub> OS; [67-68-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub> x <sub>1</sub>		
0.861 0.1	39	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METEOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.	SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	(1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-	

	28
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8] (2) Nitromethane; CH <sub>3</sub> NO <sub>2</sub> ; [75-52-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.  Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
x <sub>2</sub>	
0.996 0.004	
AUXILIARY	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not speci- fied in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not speci- fied in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ul> <li>(1) Carbazole; C<sub>12</sub>H<sub>9</sub>N; [86-74-8]</li> <li>(2) Acetic anhydride; C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>; [108-24-7]</li> </ul>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub>		
0.988 0.0	12	
AUXILIARY		
	SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-	

202		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,	
(2) 1-Methyl-2-pyrrolidinone; C <sub>5</sub> H <sub>9</sub> NO; [872-50-4]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$x_2$ $x_1$		
0.843 0.19	57	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.	
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>(1) Carbazole; C<sub>12</sub>H<sub>9</sub>N; [86-74-8]</li> <li>(2) N,N-Dimethylacetamide; C<sub>4</sub>H<sub>9</sub>NO; [127-19-5]</li> </ol>	Chernyi, A.V.; Rubstov, V.I.; Aleksandro V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
variables:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
* <sub>2</sub> * <sub>1</sub>		
0.810 0.1	90	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Carbazole; C<sub>12</sub>H<sub>9</sub>N; [86-74-8]</li> <li>(2) N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]</li> </ul>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)
VARIABLES:	PREPARED BY:
T/K = See below	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
* <sub>2</sub>	
0.836 0.164	
	INFORMATION
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.
Based upon experimental values given in the paper for solvents for which indepen- dently determined values exist, compiler estimates the temperature as between 298- 303 K.	(2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>(1) Carbazole; C<sub>12</sub>H<sub>9</sub>N; [86-74-8]</li> <li>(2) Tetramethylene sulfone; C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S; [126-33-0]</li> </ol>	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
$x_2$ $x_1$		
0.9526 0.0	174	
	TURODUARTON	
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not speci-	
METHOD: APPARATUS/PROCEDURE  No experimental details were given in the paper.  Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source not specified in paper.  (2) Purity and chemical source not speci-	

204		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbazole; C <sub>12</sub> H <sub>0</sub> N; [86-74-8]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov,	
(2) Tributyl phosphate; C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P; [126-73-8]	V.V.; Nazarov, V.N.; Vail, E.I. Sov. Prog. Chem. 1986, 52, 41-44. (English Translation)	
VARIABLES:	PREPARED BY:	
T/K = See below	W.E. Acree, Jr.	
EXPERIMENTAL VALUES		
x <sub>2</sub>		
0.911 0.089		
AUXILIARY	INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
No experimental details were given in the paper.	(1) Purity and chemical source not specified in paper.	
Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	(2) Purity and chemical source not speci- fied in paper.	
	ESTIMATED ERRORS:	
	T/K: Unknown. $x_1$ : $\pm$ 8 % (relative error; compiler).	

COMPONENTS:		ORIGINAL MEAS	SUREMENTS:
(1) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]		Cullinane, N.M.; Rees, W.T.	
(2) Dibenzofuran; C <sub>12</sub> E	1 <sub>8</sub> 0; [132-64-9]	Trans. Faraday Soc. 1940, 36, 506-51	
VARIABLES:		PREPARED BY:	
Temperature	•		Jr.
EXPERIMENTAL VALUES <sup>a</sup>			
$r_{ m in}/{ m K}$	T <sub>fin</sub> /K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>
355.6	354.7	1.000	0.000
401.6	356.7	0.898	0.102
439.2	360.7	0.753	0.247
469.5	368.6	0.562	0.438
492.8	382.7	0.331	0.669
510.0	414.4	0.141	0.859
519.0	518.3	0.000 1.000	

<sup>&</sup>lt;sup>a</sup> 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 not given, was sublimed and recrystallized from acetone.
- (2) Purity and chemical source not given in paper, was sublimed and recrystallized from alcohol several times.

## ESTIMATED ERRORS:

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

# CHRYSENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated\_Hydrocarbons (including cycloalkanes)</u>

n-heptane

- B. Alkenes
- C. Aromatic Hydrocarbons

benzene
naphthalene
anthracene
benz[a]anthracene
acenaphthene
fluorene
fluoranthene
pyrene

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

1-octanol

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

carbazole dibenzofuran

J. Binary Solvent Mixtures

	201	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]	Lissi, E.A.; Abuin, E.B.	
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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	(mol dm <sup>-3</sup> )	
20.0 0.0	0.0040	
AUXILIARY	( INFORMATION	
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:	
Constant temperature bath, centrifuge, thermometer, and an uv/visible spectrophotometer.	(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 absorbance using the Beer-Lambert law.	(2) Purity and chemical source not given, purification procedure not specified.	
	ESTINATED ERRORS:	
	$T/K$ : $\pm 2$ . $c_1$ : unknown.	

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

### COMPONENTS: ORIGINAL MEASUREMENTS: Kravchenko, V.M.; Pastukhova, I.S. (1) Chrysene; C<sub>18</sub>H<sub>12</sub>; [218-01-9] Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation) (2) Naphthalene; C10H8; [91-20-3] PREPARED BY: VARIABLES: W.E. Acree, Jr. Temperature EXPERIMENTAL VALUES T/K x<sub>2</sub> ×1 353.2 1.000 0.000 351.7 0.975 0.025 351.0 0.958 0.042 388.4 0.897 0.103 406.2 0.843 0.157 417.8 0.798 0.202 442.4 0.710 0.290 459.7 0.593 0.407 476.2 0.496 0.504 487.5 0.407 0.593 0.298 0.702 500.2 0.183 0.817 511.4 520.2 0.097 0.903 528.2 0.000 1.000 **AUXILIARY INFORMATION** METHOD: APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Phase diagram was determined using a (1) Purity and chemical source were not thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem. U.S.S.R. 1939, 13, 133), supplemented by visual observations. 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).

(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9] (2) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7]		ORIGINAL MEASUREMENTS:	
		Kravchenko, V.M.; Pastukhova, I.S.  Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)	
Temperature		W.E. Acree, Jr.	
EXPERIMENTAL VALUES			
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	
489.7	1.000	0.000	
481.7	0.897	0.103	
473.7	0.798	0.202	
469.7	0.740	0.260	
467.2	0.697	0.303	
466.2	0.635	0.365	
470.5	0.598	0.402	
480.4	0.504	0.496	
490.9	0.397	0.603	
499.7	0.307	0.693	
509.5	0.212	0.788	
519.2	0.104	0.896	
528.2	0.000	1.000	

### 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).

(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]  (2) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ;  [56-55-3]  VARIABLES:		ORIGINAL MEA	surements:		
		Sturrock, M	Sturrock, M.G.; Lawe, T.		
		Can. J. Res	Can. J. Res., Sect. B. 1939, 17, 71-74.  PREPARED BY:		
		PREPARED BY:			
Temperature		W.E. Acree,	W.E. Acree, Jr.		
EXPERIMENTAL VALUES <sup>a</sup>	<del> </del>				
$r_{in}/\mathtt{K}$	$r_{fin}/\kappa$	* <sub>2</sub>	× <sub>1</sub>		
433.2	433.2	1.00	0.00		
448.2	436.2	0.90	0.10		
470.2	442.2	0.75	0.25		
487.2	451.2	0.60	0.40		
496.2	461.2	0.50	0.50		
505.2	468.2	0.40	0.60		
516.2	484.2	0.25	0.75		
525.2	505.2	0.10	0.90		
528.2	528.2	0.00	1.00		

<sup>&</sup>lt;sup>a</sup> Continuous solid solutions were found in the chrysene - benz[a]anthracene system.  $T_{in}$  refers to the temperature at which crystallization begins;  $T_{fin}$  is the temperature at which crystallization of the solid solution concludes.

### METHOD: APPARATUS/PROCEDURE

Melting points and freezing points were obtained by determining temperatures of incipient fusion and complete liquefaction using capillary tube method. Temperature very slowly raised and material observed through a low power microscope.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Obtained from heavy crude oil, purified by column chromatography using activated alumina and recrystallized.
- (2) Obtained from heavy crude oil, and was fractionally recrystallized from alcohol before use.

### ESTIMATED ERRORS:

T/K: precision  $\pm$  0.5 (Compiler).  $x_1$ :  $\pm$  0.005 (Compiler).

COMPONENTS:		ORIGINAL MEA	SUREMENTS:	
(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9] (2) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ; [56-55-3]		Kravchenko, V.M.; Pastukhova, I.S.  Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)		
Temperature		W.E. Acree,	Jr.	
EXPERIMENTAL VALUES <sup>3</sup>				
$r_{in}/\kappa$	$T_{\sf fin}/{\tt K}$	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	
431.2	430.9	1.000	0.000	
435.4	431.7	0.960	0.040	
438.2	432.2	0.947	0.053	
446.7	434.2	0.898	0.102	
451.6	436.2	0.852	0.148	
459.2	438.6	0.805	0.195	
473.8	445.2	0.700	0.300	
483.2	453.2	0.603	0.397	
493.7	461.7	0.498	0.502	ļ
502.2	474.2	0.395	0.605	
508.7	486.2	0.300	0.700	
514.5	499.2	0.202	0.798	Ì
522.2	513.2	0.095	0.905	
528.2	528.2	0.000	1.000	
				[

<sup>&</sup>lt;sup>a</sup> Continuous solid solutions were found in the chrysene - benz[a]anthracene system.  $T_{\rm in}$  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

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) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9] (2) Acenaphthene; C <sub>12</sub> H <sub>10</sub> ; [83-32-9]  VARIABLES: Temperature		Kravchenko, V.M.; Pastukhova, I.S.  Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)	
		W.E. Acree, Jr.	
		EXPERIMENTAL VALUES	
T/K	<i>x</i> <sub>2</sub>	$x_{1}$	
368.2	1.000	0.000	
366.4	0.966	0.034	
364.2	0.928	0.072	
378.5	0.899	0.101	
416.2	0.796	0.204	
437.4	0.704	0.296	
457.0	0.596	0.404	
471.5	0.499	0.501	
477.8	0.387	0.613	
500.2	0.278	0.722	
513.2	0.147	0.853	
528.2	0.000	1.000	
		INFORMATION	
METHOD: APPARATUS/PROCE		SOURCE AND PURITY OF MATERIALS:	
Phase diagram was determined thermal analysis method detail in V.M. Kravcher U.S.S.R. 1939, 13, 13	d (described in the land) in the land of t	(1) Purity and chemical source were not specified in paper, was recrystallized before use.	
visual observations.		(2) Purity and chemical source were not specified in paper, was recrystallized before use.	
		ESTIMATED ERRORS:	
		$T/K$ : precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).	

ORIGINAL MEASUREMENTS:  Kravchenko, V.M.; Pastukhova, I.S.  Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)  PREPARED BY:  W.E. Acree, Jr.   X1  0.000  0.052  0.098  0.129  0.205  0.320  0.403  0.555  0.650  0.754  0.861  1.000
### Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)  PREPARED BY:  W.E. Acree, Jr.   **1  0.000  0.052  0.098  0.129  0.205  0.320  0.403  0.555  0.650  0.754  0.861
1956, 111, 667-669 (English translation)  PREPARED BY:  W.E. Acree, Jr.   x <sub>1</sub> 0.000 0.052 0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754 0.861
<pre>x<sub>1</sub> 0.000 0.052 0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754 0.861</pre>
x <sub>1</sub> 0.000 0.052 0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754 0.861
0.000 0.052 0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754
0.000 0.052 0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754
0.052 0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754
0.098 0.129 0.205 0.320 0.403 0.555 0.650 0.754
0.129 0.205 0.320 0.403 0.555 0.650 0.754 0.861
0.205 0.320 0.403 0.555 0.650 0.754 0.861
0.320 0.403 0.555 0.650 0.754 0.861
0.403 0.555 0.650 0.754 0.861
0.555 0.650 0.754 0.861
0.650 0.754 0.861
0.754 0.861
0.861
1.000
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:  Kravchenko, V.M.; Pastukhova, I.S.  Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, 111, 667-669 (English translation)		
(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]			
(2) Fluoranthene; C <sub>16</sub> H <sub>10</sub> ; [206-44-0]			
VARIABLES:	PREPARED BY:		
Temperature	W.E. Acree, Jr.		
EXPERIMENTAL VALUES			
<i>T</i> /K	$x_1$		
383.2 1.000	0.000		
378.7 0.939	0.061		
378.2 0.918	0.082		
387.3 0.897	0.103		
403.2 0.846	0.154		
418.8 0.799	0.201		
442.4 0.691	0.309		
457.2 0.602	0.398		
474.5 0.498	0.502		
486.2 0.404	0.596		
498.4 0.293	0.707		
510.5 0.195	0.805		
519.2 0.090	0.910		
528.2 0.000	1.000		
AUXILIAN METHOD: APPARATUS/PROCEDURE  Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, J. Phys. Chem.	SOURCE AND PURITY OF MATERIALS:  (1) Purity and chemical source were not specified in paper, was recrystallized before use.		
U.S.S.R. 1939, 13, 133), supplemented by visual observations.	(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
	ESTIMATED ERRORS:		
	T/K: precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).		

COMPONENTS:  (1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]  (2) Pyrene; C <sub>16</sub> H <sub>10</sub> ; [129-00-0]  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	<b>*</b> 2	<i>x</i> <sub>1</sub>	
423.2	1.000	0.000			
413.7	0.901	0.099			
410.2	0.864	0.136			
408.2	0.835	0.165			
415.4	0.813	0.187			
420.6	0.790	0.210			
441.2	0.697	0.303			
458.7	0.602	0.398			
473.2	0.505	0.495			
487.2	0.396	0.604			
496.2	0.314	0.686			
506.7	0.218	0.782			
517.7	0.103	0.897			
528.2	0.000	1.000			
		INFORMATION			
METHOD: APPARATUS/PROCE	DURE	SOURCE AND PURITY OF MATERIALS:			
Phase diagram was dete thermal analysis metho detail in V.M. Kravche U.S.S.R. 1939, 13, 13	d (described in nko, J. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.			
visual observations.	••	(2) Purity and chemical source were not specified in paper, was recrystallized before use.			
		ESTIMATED ERRORS:			
		$T/K$ : precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]	Miller, M.M.; Wasik, S.P.; Huang, GL.; Shiu, WY.; Mackay, D.
(2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]	Environ. Sci. Technol. 1985, 19, 522-529.
VARIABLES:	PREPARED BY:
T/K = 298	W.E. Acree, Jr.
EXPERIMENTAL VALUES	
t/°C	(mol dm <sup>-3</sup> )
25.0 0.0	0200
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:
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9] (2) Carbazole; C <sub>12</sub> H <sub>9</sub> N; [86-74-8]  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	<b>x</b> <sub>2</sub>	x <sub>1</sub>		
517.2	1.000	0.000		
507.5	0.892	0.108		
499.2	0.800	0.200		
489.6	0.699	0.301		
484.7	0.653	0.347		
479.8	0.604	0.396		
477.2	0.555	0.445		
478.4	0.528	0.472		
482.9	0.495	0.505		
493.4	0.394	0.606		
500.7	0.302	0.698		
511.2	0.195	0.805		
519.7	0.097	0.903		
528.2	0.000	1.000		
	AUXILIARY	INFORMATION	-	
METHOD: APPARATUS/PROCEI	OURE	SOURCE AND PURITY OF MATERIALS:	_	
Phase diagram was deter thermal analysis method detail in V.M. Kravcher U.S.S.R. 1939, 13, 13	d (described in nako, J. Phys. Chem.	(1) Purity and chemical source were not specified in paper, was recrystallized before use.	ļ	
visual observations.	of, embhremented by	(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
		ESTIMATED ERRORS:	_	
		$T/K$ : precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).		

COMPONENTS:  (1) Chrysene; C <sub>18</sub> H <sub>12</sub> ; [218-01-9]  (2) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9]  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	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>
356.2	1.000	0.000		
354.7	0.968	0.032		
353.2	0.940	0.060		
373.7	0.907	0.093		
401.2	0.848	0.152		
429.2	0.752	0.248		
450.4	0.649	0.351		
474.6	0.496	0.504		
486.7	0.404	0.596		
499.0	0.300	0.700		
509.6	0.295	0.805		
516.5	0.113	0.887		
528.2	0.000	1.000		
METHOD: APPARATUS/PROCE		SOURCE AND PURITY OF MATERIALS:		
Phase diagram was dete thermal analysis metho detail in V.M. Kravche	rmined using a d (described in	(1) Purity and chemical source were not specified in paper, was recrystallized before use.		
U.S.S.R. 1939, 13, 13 visual observations.	3), supplemented by	(2) Purity and chemical source were not specified in paper, was recrystallized before use.		
		ESTIMATED ERRORS:		
		$T/K$ : precision $\pm$ 0.2 (Compiler). $x_1$ : $\pm$ 0.002 (Compiler).		

# CORONENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

- B. Alkenes
- C. Aromatic Hydrocarbons
- 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

<del>, , , , , , , , , , , , , , , , , , , </del>						
COMPONENTS:	ORIGINAL MEASUREMENTS:					
(1) Coronene; C <sub>24</sub> H <sub>12</sub> ; [191-07-1]	Lissi, E.A.; Abuin, E.B.					
(2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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	(mol dm <sup>-3</sup> )					
20.0 0.00048						
AUXILIARY	INFORMATION					
METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:					
Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.	(1) Purity not given, commercial sample of unspecified source, was used as received.					
Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured fluorescence emission intensity.	(2) Purity and chemical source not given, purification procedure not specified.					
	ESTIMATED ERRORS:					
	$T/K$ : $\pm 2$ . $c_1$ : unknown.					

COMPONENTS:  (1) Coronene; C <sub>24</sub> H <sub>12</sub> ; [191-07-1]  (2) 1-Octanol; C <sub>8</sub> H <sub>18</sub> O; [111-87-5]  VARIABLES:  T/K = 298	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	(mol dm <sup>-3</sup> )			
25.0 0.000386				
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:			
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).			

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

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

1-octanol

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

302					
COMPONENTS:	ORIGINAL MEASUREMENTS:				
(1) Dibenz[a,h]anthracene; C22H14;	Lissi, E.A.; Abuin, E.B.				
[53-70-3] (2) n-Heptane; C <sub>7</sub> H <sub>16</sub> ; [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	(mol dm <sup>*3</sup> )				
20.0 0.00034					
	SOURCE AND PURITY OF MATERIALS:				
AUXILIARY METHOD: APPARATUS/PROCEDURE  Constant temperature bath, centrifuge,	SOURCE AND PURITY OF MATERIALS:  (1) Purity not given, commercial sample of				
thermometer, and an uv/visible spectro- photometer.	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 absorbance using the Beer-Lambert law.	(2) Purity and chemical source not given, purification procedure not specified.				
	ESTIMATED ERRORS:				
	$T/K$ : $\pm 2$ . $c_1$ : unknown.				

COMPONENTS:	ORIGINAL MEASUREMENTS:				
<pre>(1) Dibenz[a,h]anthracene; C<sub>22</sub>H<sub>14</sub>;     [53-70-3] (2) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]</pre>	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					
t/°C	mol dm <sup>-3</sup> )				
25.0 0.00	00938				
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:				
	$T/K$ : $\pm$ 0.1 (compiler). $c_1$ : $\pm$ 3 % (relative error; compiler).				

### DIBENZOFURAN SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane decahydronaphthalene

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

benzene
1,2,3,4-tetrahydronaphthalene

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

pyridine thiophene

J. Binary Solvent Mixtures

304	<del></del>		L ARTATURE A			
(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]			ORIGINAL MEASUREMENTS:  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	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	
327.8	0.5774	0.4226	338.5	0.3300	0.6700	
330.2	0.5195	0.4805	345.1	0.1880	0.8120	
334.0	0.4564	0.5436				
337.5	0.3700	0.6300			•	
		AUXILIARY	INFORMATION	₹		
METHOD: APPAR	ATUS/PROCEDUR	Œ	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		<ul> <li>(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.</li> <li>(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.</li> </ul>				
increased. S	olubility det	ermined by	ESTIMATED	ERRORS:		
	noting the temperature at which the last trace of solid solute disappeared.			T/Y: precision + 0.1		

COMPONENTS:			ORIGINAL MEA	ORIGINAL MEASUREMENTS:			
(1) Dibenzof (132-64-	(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O;			Auwaerter	J.E.; McLaughlin, E.		
(2) Decahydr [91-17-8	onaphthalene;	C <sub>10</sub> H <sub>18</sub> ;	Fluid Phase	Fluid Phase Equilibr. 1			
VARIABLES:			PREPARED BY:				
Temperature			W.E. Acree,	Jr.			
EXPERIMENTAL	VALUES						
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<b>x</b> <sub>1</sub>		
326.4	0.5755	0.4245	337.2	0.3553	0.6447		
328.2	0.5354	0.4646					
331.5	0.4890	0.5110					
	0.4248	0.5752					

METHOD: APPARATUS/PROCEDURE

thermometer.

Constant temperature bath and a precision

Mixtures of known concentrations sealed

in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly

increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

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

SOURCE AND PURITY OF MATERIALS:

ESTIMATED ERRORS:

 $x_1$ :  $\pm 0.0003$ .

T/K: precision  $\pm$  0.1.

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from solution.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 %

trans, stored over molecular sieves.

COMPONENTS:	······································	ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]		Domanska, U.; Groves, F.R., Jr.; McLaughlin, E.  J. Chem. Eng. Data 1993, 38, 88-94.			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>			
278.7	1.0000	0.0000			
276.1	0.9365	0.0635			
274.0	0.9144	0.0856			
273.4	0.9066	0.0934			
272.4	0.8878	0.1122			
274.8	0.8761	0.1239			
277.9	0.8637	0.1363			
280.2	0.8537	0.1463			
282.8	0.8401	0.1599			
290.3	0.8022	0.1978			
296.3	0.7654	0.2346			
298.3	0.7520	0.2480			
302.5	0.7187	0.2813			
305.3	0.7005	0.2995			
312.0	0.6441	0.3559			
320.0	0.5514	0.4486			
329.1	0.4209	0.5791			
337.7	0.2955	0.7045			
340.9	0.2430	0.7570			
346.4	0.1654	0.8346			
355.3	0.0000	1.0000			

### 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 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:

			<del>,</del>			
Components:			ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.				
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]			J. Solution Chem. 1988, 16, 519-534.			
VARIABLES:			PREPARED I	SY:		
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL \	ALUES		<del> </del>			
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	
321.9	0.5203	0.4797	338.7	0.2776	0.7224	
323.5	0.4932	0.5068				
329.4	0.4156	0.5844				
332.0	0.3778	0.6222				
		AUXILIARY	INFORMATION	ī		
METHOD: APPARA	TUS/PROCEDUR	E	SOURCE ANI	PURITY OF M	ATERIALS:	
thermometer.	•	and a precision	(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.				
noting the te	emperature at	which the last	ESTIMATED	ERRORS:		
frace or soll	trace of solid solute disappeared.		T/K: precision ± 0.1. x <sub>1</sub> : ± 0.0003.			

COMPONENTS:			ORIGINAL MEASUREMENTS:  Coon, J.E.; Auwaerter, J.E.; McLaughlin, E			
(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9]						
(2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2]			Fluid Phase Equilibr. 1989, 44, 305-345.			
VARIABLES:	RIABLES:			BY:		
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	
318.9	0.5479	0.4521	339.5	0.2670	0.7330	
322.6	0.5093	0.4907				
326.6	0.4506	0.5494				
337.9	0.3010	0.6990				
		AUXILIARY	INFORMATION			
ETHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
thermometer.	nt temperature bath and a precision meter.			(1) 99.6 %, Aldrich Chemical Company, Mil waukee, Wisconsin, USA, was recrystal from solution.		
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		store		Chemical Company, was cular sieves to remove		
noting the to	emperature at	which the last	ESTIMATED	ERRORS:	· · · · · · · · · · · · · · · · · · ·	
trace of solid solute disappeared.			T/K: precision ± 0.1.			

COMPONENTS:	COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.					
					<u>88</u> , <i>16</i> , 519-534.		
VARIABLES:	VARIABLES:		PREPARED E	Y:			
Temperature	Temperature		W.E. Acre	e, Jr.			
EXPERIMENTAL '	VALUES	· · · · · · · · · · · · · · · · · · ·	ļ				
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x2	<b>x</b> <sub>1</sub>		
323.7	0.4917	0.5083	340.8	0.2418	0.7582		
326.2	0.4554	0.5446					
331.2	0.3839	0.6161					
336.3	0.3188	0.6812					
		AUXILIARY	YINFORMATION				
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
Constant temperature bath and a precision thermometer.			(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene.				
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.					
noting the te	emperature at	which the last	ESTIMATED	ERRORS:			
trace or sol:	fa solace als	appeared.	$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003.				

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzofuran; C <sub>12</sub> H <sub>8</sub> O; [132-64-9] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.			
VARIABLES:	ARTARLES:			Y:		
Temperature				PREPARED BY: W.E. Acree, Jr.		
EXPERIMENTAL '	VALUES					
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	<i>*</i> 1	
314.2	0.5780	0.4220	337.0	0.3040	0.6960	
319.3	0.5243	0.4757	341.1	0.2415	0.7585	
322.3	0.4917	0.5083				
332.8	0.3653	0.6347				
		AUXILIARY	INFORMATION			
METHOD: APPARA	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			kee, from (2) Gold Compa	Wisconsin, U toluene. Label, 99.9+ ny, was used	mical Company, Milwau- SA, was recrystallized %, Aldrich Chemical as received.	
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			ESTIMATED $T/K: prec   x_1: \pm 0.0$	ision ± 0.1.		

### DIBENZOTHIOPHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane decahydronaphthalene

- B. Alkenes
- C. Aromatic Hydrocarbons

benzene
1,2,3,4-tetrahydronaphthalene

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

pyridine thiophene

J. Binary Solvent Mixtures

COMPONENTS:	COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzothiophene; C <sub>12</sub> H <sub>8</sub> S; [132-65-0] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]		Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.					
					88, 10, 519-534.		
VARIABLES:	RIABLES:		PREPARED F	3Y:			
Temperature			W.E. Acre	e, Jr.			
EXPERIMENTAL '	VALUES		<del> </del>				
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	$x_1$		
320.6	0.9129	0.0871	343.0	0.6846	0.3154		
326.6	0.8871	0.1129	343.3	0.6654	0.3346		
328.2	0.8706	0.1294					
335.8	0.8001	0.1999					
		AUXILIARY	INFORMATION	ī			
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:		
thermometer.				(1) 99 %, Aldrich Chemical Company, Milwau- kee, Wisconsin, USA, was recrystallized from toluene.			
Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by		(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.					
noting the to	emperature at	which the last	ESTIMATED	ERRORS:			
trace of solid solute disappeared.		T/K: precision ± 0.1. x,: ± 0.0003.					

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzothiophene; C <sub>12</sub> H <sub>8</sub> S; [132-65-0] (2) Decahydronaphthalene; C <sub>10</sub> H <sub>18</sub> ; [91-17-8]  VARIABLES:			Fluid Pha	se Equilibr. Y:	., J.E.; McLaughlin, E. 1989, 44, 305-345.	
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL '	VALUES		· · · · · · · · · · · · · · · · · · ·			
T/K	*2 0.8944	* <sub>1</sub> 0.1056	<i>T/K</i> 333.9	x <sub>2</sub> 0.7372	x <sub>1</sub> 0.2628	
318.9	0.8607	0.1393				
325.8	0.8141	0.1859				
		AUXILIARY	INFORMATION			
METHOD: APPAR	ATUS/PROCEDUR	Ε	SOURCE AND	PURITY OF M	MATERIALS:	
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			wauke lized (2) 99+ % isome trans	e, Wisconsin from soluti , Aldrich Ch r ratio of 6 , stored ove	Chemical Company, Mil- n, USA, was recrystal- on. Demical Company, having 10.6 % cis and 39.4 % or molecular sieves.	
			ESTIMATED ERRORS: $T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003.			

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Dibenzothiophene; [132-65-0]		Domanska, U.; Groves, F.R., Jr.; McLaughlin E.			
(2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-	-43-2]	J. Chem. Eng. Data <u>1993</u> , 38, 88-94.			
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES	· <del> · · · · · · · · · · · · · · · · ·</del>				
T/K	* <sub>2</sub>	<b>x</b> <sub>1</sub>			
278.7	1.0000	0.0000			
278.0	0.9770	0.0230			
277.2	0.9570	0.0430			
276.6	0.9468	0.0532			
276.0	0.9402	0.0598			
278.2	0.9337	0.0663			
283.1	0.9216	0.0784			
285.7	0.9133	0.0867			
290.5	0.8990	0.1010			
294.7	0.8842	0.1152			
299.2	0.8670	0.1330			
301.3	0.8571	0.1429			
304.3	0.8427	0.1573			
306.7	0.8301	0.1699			
312.9	0.7934	0.2066			
319.2	0.7884	0.2516			
325.6	0.6962	0.3038			
330.7	0.6399	0.3601			
335.4	0.5869	0.4131			
340.8	0.5267	0.4733			
346.4	0.4649	0.5351			
350.3	0.4142	0.5858			
353.2	0.3577	0.6423			
372.0	0.0000	1.0000			
	AUXILI	TARY INFORMATION			

# METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

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

### SOURCE AND PURITY OF MATERIALS:

- 99 %, Aldrich Chemical Company, Milwau-kee, Wisconsin, USA, was recrystallized from toluene.
- (2) 99+ %, Aldrich Chemical Company, was fractionally distilled and stored over molecular sieves.

# ESTIMATED ERRORS:

						0.
COMPONENTS:  (1) Dibenzothiophene; C <sub>12</sub> H <sub>8</sub> S; [132-65-0] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]			ORIGINAL MEASUREMENTS:  Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.			
						VARIABLES:
Temperature						
EXPERIMENTAL '	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>	
309.9	0.8104	0.1896	342.3	0.4856	0.5144	
315.3	0.7754	0.2246				
327.8	0.6653	0.3347				
337.2	0.5638	0.4362				
		AUXILIARY	INFORMATION	ī		
METHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	<del></del>
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			kee, from (2) Gold	Wisconsin, U. toluene.  Label, 99.9+	mical Company, Mi SA, was recrystal %, Aldrich Chemi as received.	llized
			ESTIMATED ERRORS:			
			T/K: pred x <sub>1</sub> : ± 0.0	ision ± 0.1.		

(1) Dibenzothiophene; C <sub>12</sub> H <sub>8</sub> S; [132-65-0] (2) 1,2,3,4-Tetrahydronaphthalene; C <sub>10</sub> H <sub>12</sub> ; [119-64-2]			ORIGINAL MEASUREMENTS:  Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.  Fluid Phase Equilibr. 1989, 44, 305-345.			
						VARIABLES:
Temperature			W.E. Acree, Jr.			
EXPERIMENTAL	VALUES					
T/K	×2	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	
308.7	0.7837	0.2163	337.8	0.5308	0.4692	
318.2	0.7219	0.2781				
326.6	0.6492	0.3508				
336.3	0.5534	0.4466				
		AUXILIARY	INFORMATION			
ETHOD: APPAR	ATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	MATERIALS:	
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			<ul> <li>(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystal-from solution.</li> <li>(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.</li> <li>ESTIMATED ERRORS:</li> <li>T/K: precision + 0.1.</li> </ul>			

COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Dibenzothiophene; C <sub>12</sub> H <sub>8</sub> S; [132-65-0] (2) Pyridine; C <sub>5</sub> H <sub>5</sub> N; [110-86-1] 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	EXPERIMENTAL VALUES					
T/K	×2	<i>x</i> <sub>1</sub>	T/K	x <sub>2</sub>	$x_{1}$	
306.5	0.7857	0.2143	334.7	0.5502	0.4498	
313.0	0.7448	0.2552	335.2	0.5348	0.4652	
322.8	0.6687	0.3313				
327.4	0.6216	0.3784		•		
		AUXILIARY	INFORMATION			
METHOD: APPARA	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 noting the temperature at which the last trace of solid solute disappeared.			kee, from (2) Gold	Wisconsin, U toluene. Label, 99.9+	mical Company, Milwau- SA, was recrystallized %, Aldrich Chemical as received.	
			T/K: prec	cision <u>+</u> 0.1.		

COMPONENTS:  (1) Dibenzothiophene; C <sub>12</sub> H <sub>8</sub> S; [132-65-0] (2) Thiophene; C <sub>4</sub> H <sub>4</sub> S; [110-02-1]  VARIABLES: Temperature			ORIGINAL MEASUREMENTS:			
			Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E. McLaughlin, E.  J. Solution Chem. 1988, 16, 519-534.			
			PREPARED B	Y:		
			W.E. Acree, Jr.			
EXPERIMENTAL '	VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>*</i> 1	T/K	*2	× <sub>1</sub>	
309.3	0.7621	0.2379	328.1	0.6128	0.3872	
315.2	0.7224	0.2776	337.0	0.5050	0.4950	
322.7	0.6639	0.3361				
327.0	0.6257	0.3743				
		AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROCEDURE			SOURCE AND PURITY OF MATERIALS:			
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by			(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.  (2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.			
						noting the temperature at which the last trace of solid solute disappeared.

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

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

benzene

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

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) 1,2-Diphenylbenzer	ne; C <sub>18</sub> H <sub>14</sub> ;	McLaughlin, E.; Zainal, H.A.			
[84-15-1] (2) Cyclohexane; C <sub>6</sub> H <sub>12</sub>	; [110-82-7]	J. Chem. Soc. <u>1960</u> , 3854-3857.			
, , , ,					
VARIABLES:		PREPARED BY:			
Temperature		W.E. Acree, Jr.			
EXPERIMENTAL VALUES					
T/K	<b>x</b> <sub>2</sub>	<i>x</i> <sub>1</sub>			
296.0	0.6463	0.3537			
303.2	0.5004	0.4996			
313.6	0.2927	0.7073			
322.8 0.1045		0.8955			
	AUXILIARY	INFORMATION			
METHOD: APPARATUS/PROC	EDURE	SOURCE AND PURITY OF MATERIALS:			
Constant temperature I thermometer.	path and a precision	(1) Purity not given, Eastman Kodak, Roches- ter, New York, USA, was passed over an alumina column with light petroleum			
Mixtures of known cond		ether as eluant. (2) Purity, source, and purification method			
in glass ampoules and temperature to equili	brate. Samples	were not specified.			
were rotated while bat increased. Solubility	determined by				
noting the temperature trace of solid solute		ESTIMATED ERRORS:			
		$T/K$ : precision $\pm$ 0.1. $x_i$ : $\pm$ 0.0003 (compiler).			
1		1 x1. ± 0.0003 (compiler).			

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) 1,2-Diphenylbenzend [84-15-1] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-		McLaughlin, E.; Zainal, H.A.  J. Chem. Soc. <u>1959</u> , 863-867.		
VARIABLES:		PREPARED BY:		
Temperature		W.E. Acree, Jr.		
EXPERIMENTAL VALUES				
T/K	<i>x</i> <sub>2</sub>	x <sub>1</sub>		
301.2	0.4148	0.5852		
305.6	0.3558	0.6442		
318.0	0.1898	0.8102		
323.6	0.0987	0.9013		
	AUXILIARY	INFORMATION		
METHOD: APPARATUS/PROCES	OURE	SOURCE AND PURITY OF MATERIALS:		
Constant temperature be thermometer.  Mixtures of known concein glass ampoules and ptemperature to equilibrate were rotated while bath increased. Solubility of	entrations sealed placed in constant rate. Samples n temperature slowly	(1) Purity not given, Eastman Kodak, Rochester, New York, USA, was passed over an alumina column with light petroleum ether as eluant.  (2) "AnalaR", was dried over sodium wire and freshly distilled before use.		
noting the temperature trace of solid solute of	at which the last	ESTIMATED ERRORS:  T/K: precision ± 0.1.  x <sub>1</sub> : ± 0.0003 (compiler).		

(1) 1,2-Diphenylbenzene; C <sub>18</sub> H <sub>14</sub> ; [84-15-1] (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]			ORIGINAL MEASUREMENTS:		
			McLaughlin, E.; Zainal, H.A.  J. Chem. Soc. 1960, 2485-2488.		
VARIABLES:			PREPARED F	BY:	
Temperature			W.E. Acre	ee, Jr.	
EXPERIMENTAL '	VALUES				
T/K	<b>x</b> <sub>2</sub>	$x_1$	T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>
302.0	0.4257	0.5743	323.0	0.1125	0.8875
308.0	0.3293	0.6707			
314.8	0.2507	0.7493			
318.6	0.1814	0.8186			
		AUXILIARY	INFORMATION	<b>1</b>	
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		<ol> <li>Purity not given, Eastman Kodak, Roche ter, New York, USA, was passed over an alumina column with light petroleum ether as eluant.</li> <li>AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.</li> </ol>			
increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			ERRORS: cision ± 0.1.		

1.3-r	IPHENYLBENZENE	SOLUBILITIES	IN PURE	AND RINARY	SOLVENT	MIXTURES

- A. Saturated Hydrocarbons (including cycloalkanes)

  cyclohexane
- B. Alkenes
- C. Aromatic Hydrocarbons

benzene

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

					O.	
COMPONENTS:  (1) 1,3-Diphenylbenzene; C <sub>18</sub> H <sub>14</sub> ;		ORIGINAL N	MEASUREMENTS:			
		McLaughlin, E.; Zainal, H.A.				
[92-06-8 (2) Cyclohex	} ane; C <sub>6</sub> H <sub>12</sub> ; []	110-82-7]	J. Chem.	Soc. 1960,	3854-3857.	
VARIABLES:			PREPARED BY:			
Temperature			W.E. Acre	ee, Jr.		
EXPERIMENTAL	VALUES		-			
T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>*</i> 1	
311.4	0.9230	0.0770	333.4	0.5925	0.4075	
320.6	0.8368	0.1632				
325.5	0.7579	0.2421				
329.9	0.6669	0.3331				
		AUXILIARY	INFORMATIO	Ą		
METHOD: APPAR	ATUS/PROCEDUR	Œ	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		Unite alum ether (2) Puri	ed Kingdom, w ina column wi r as eluant.	British Drug Houses, as passed over an th light petroleum d purification method		
noting the t	emperature at	which the last	ESTIMATED			
trace of solid solute disappeared.			$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003 (compiler).			

COMPONENTS:		ORIGINAL MEASUREMENTS:					
(1) 1,3-Diphe [92-06-8	(1) 1,3-Diphenylbenzene; C <sub>18</sub> H <sub>14</sub> ;		McLaughli	McLaughlin, E.; Zainal, H.A.			
(2) Benzene;	C <sub>6</sub> H <sub>6</sub> ; [71-43	-2]	J. Chem.	Soc. <u>1959</u> ,	863-867.		
VARIABLES:			PREPARED I	BY:	<del></del>		
Temperature		W.E. Acre	ee, Jr.				
EXPERIMENTAL '	VALUES					<del>_</del>	
T/K	<b>x</b> <sub>2</sub>	<b>x</b> <sub>1</sub>	T/K	<i>x</i> <sub>2</sub>	<i>x</i> <sub>1</sub>		
310.0	0.7173	0.2827	347.4	0.2429	0.7571		
320.2	0.6162	0.3838	350.8	0.1656	0.8344		
334.0	0.4534	0.5466					
340.6	0.3593	0.6407					

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

Constant temperature bath and a precision

METHOD: APPARATUS/PROCEDURE

thermometer.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with light petroleum
- ether as eluant.
  (2) "AnalaR", was dried over sodium wire and freshly distilled before use.

#### ESTIMATED ERRORS:

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

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) 1,3-Diphenylbenzene; C <sub>18</sub> H <sub>14</sub> ; [92-06-8] (2) Tetrachloromethane; CCl <sub>4</sub> ; [56-23-5]		McLaughlin, E.; Zainal, H.A.  J. Chem. soc. <u>1960</u> , 2485-2488.			
/ARIABLES:	PREPARED BY: W.E. Acree, Jr.				
Temperature					
EXPERIMENTAL VALUES					
T/K ×2	<b>x</b> <sub>1</sub>	T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>	
312.6 0.7937	0.2063	343.2	0.5750	0.4250	
318.2 0.7391	0.2609				
328.6 0.6282	0.3718				
	AUXILIARY	INFORMATION	T		
METHOD: APPARATUS/PROCEDUR	E	SOURCE AND	PURITY OF M	ATERIALS:	
Constant temperature bath thermometer.  Mixtures of known concents in glass ampoules and plattemperature to equilibrate were rotated while bath to increased. Solubility detending the temperature at	Unite alumi ether (2) Anala dried	d Kingdom, w na column wi as eluant. R grade, sou l over anhydr listilled bef	British Drug Houses, as passed over an th light petroleum rce not given, was ous calcium chloride ore use.		
trace of solid solute dis		ision ± 0.1.	r).		

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

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

benzene

- 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

COMPONENTS:	COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) 1,4-Diphenylbenzene; C <sub>18</sub> H <sub>14</sub> ; [92-94-4] (2) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]			McLaughlin, E.; Zainal, H.A.  J. Chem. Soc. <u>1959</u> , 863-867.			
VARIABLES:	<del>,</del>		PREPARED B	Y:		
Temperature	Temperature			e, Jr.		
EXPERIMENTAL V	ALUES		<u> </u>	<del>" " " " " " " " " " " " " " " " " " " </del>		
T/K	x <sub>2</sub>	<i>x</i> <sub>1</sub>	T/K	* <sub>2</sub>	<i>x</i> <sub>1</sub>	
311.2	0.9929	0.0071	350.8	0.9721	0.0279	
333.4	0.9844	0.0156				
337.4	0.9822	0.0178				
341.2	0.9796	0.0204			•	
		AUXILIARY	INFORMATION	4		
METHOD: APPAR	ATUS/PROCEDUR	Œ	SOURCE AND	D PURITY OF I	MATERIALS:	
Constant temperature bath and a precision thermometer.  Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples			<ul><li>(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.</li><li>(2) "AnalaR", was dried over sodium wire and freshly distilled before use.</li></ul>			
increased. S	temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.			ERRORS:		
			$T/K$ : precision $\pm$ 0.1. $x_1$ : $\pm$ 0.0003 (compiler).			

## SYSTEM INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

Acenaphthene		
	anthracene	12
	benzene	4
	chrysene	15
	cyclohexane	2, 3
	decahydronaphthalene	3
<u>*</u>	1,2-dimethylbenzene	6
	2,6-dimethylnaphthalene	10
	2,7-dimethylnaphthalene	11
	ethanol	18
	fluoranthene	16
	fluorene	14
	methanol	18
	methylbenzene	5
	2-methylnaphthalene	9
	naphthalene	8
	octadecane	2
	1-octanol	19
	phenanthrene	13
	1-propanol	19
	pyridine	20
	tetrachloromethane	17
	1,2,3,4-tetrahydronaphthalene	5
	1,2,4,5-tetramethylbenzene	7
	1,2,3,5-tetranitrobenzene	21
	thiophene	20
+	trichloromethane	17
1 . 1		
Acridine	<b>h</b>	
	benzene	24
	cyclohexane	23
	decahydronaphthalene	23
	pyridine	25
	1,2,3,4-tetrahydronaphthalene	24
+	thiophene	25
Anthracene		
	acenaphthene	44
	acetic anhydride	73
	acetonitrile	71, 141
	aniline	76
	benzene	37-41
	bromobenzene	59
	1-butanol	63, 64, 99-105, 134,
•	2 24041102	138
+	2-butanol	64, 106-112, 135,
•	2 Datanol	
+	2-butanone	139, 140 71
+		36, 84, 91, 98, 105,
τ	- westroloronovene	112, 119, 126, 133
+	butyl ethanoate	48
	carbon disulfide	72
	chlorobenzene	59, 60
+	1-chlorobutane	57
+	chrysene	45
+	cyclohexane	32, 33, 88, 95, 102,
		109, 116, 123, 130
		• • •

Anthracene	+ cyclooctane	34
	+ decahydronaphthalene	
	+ dibutyl oxalate	37 49
	+ 1,4-dichlorobutane	57
	+ diethyl hexanedicate	49
	+ N,N-dimethylacetamide	80
	+ 1,4-dimethylbenzene	42, 43
	+ N,N-dimethylformamide	80
	+ dimethyl hexanedloate	48
	+ dimethyl sulfoxide	
	+ 1,4-dioxane	73, 74, 144
	+ ethyl ethanoate	53, 54 47
	+ fluoranthene	46
	+ heptane	
	· ···cpound	30, 86, 93, 100, 107,
	+ hexadecane	114, 121, 128
	+ hexane	31
		29, 85, 92, 99, 106,
	+ 1-hydroxy-2-methylbenzene	113, 120, 127
	+ iodobenzene	69
	+ iodoethane	58
	+ methanol	56
	+ methoxybenzene	60, 61, 142
	+ methylbenzene	79
	+ 3-methyl-1-butanol	41, 42
	+ methylcyclohexane	65, 120-126
	methylogotomekane	34, 89, 96, 103, 110,
	+ 2-methyl-1-propanol	117, 124, 131
	+ 1-methyl-2-pyrrolidinone	65, 113-119
	+ nitrobenzene	79
	+ Octadecane	74, 75
	+ octane	32
	+ Occasie	31, 87, 94, 101, 108,
	+ 1-octanol	115, 122, 129
	1 -Octanor	66-68, 127-133, 137,
	+ 1,1-oxybisbutane	140
	+ 1,1-oxybisethane	50, 51
	<del>-</del>	50
	+ phenol + lepropago	68
	+ 1-propanol + 2-propanol	62, 85-91, 134-137
	+ 2-propanol	63, 92-98, 136, 138,
	+ 2-propanono	139, 143
	+ 2-propanone	69, 70
	+ 4-isopropyl methylbenzene	43
	+ pyridine + quinoline	76, 77
		78
	+ 2,6,10,15,19,23-hexamethyltetracosane	
	+ totrachlorovethere	36
	+ tetrachloromethane	55, 56
	+ tetrahydrofuran	52
	+ 1,2,3,4-tetrahydronaphthalene	47
	+ tetrahydropyran	52
	+ tetramethylene sulfone	81
	+ 1,2,3,5-tetranitrobenzene	82
	+ thiophene	78
	+ tributyl phosphate	81
	+ trichloroethylene	58
	+ trichloromethane	54, 55
	+ 2,2,4-trimethylpentane	35, 84, 90, 97, 104
		111, 118, 125, 13
	+ 2,4,6-trinitrophenol	83
	+ water	141-144
		= =
Benz[a]anthracene		
	+ heptane	146
Benzo[b]fluorene		
Benzo[b]fluorene	+ 1-octanol	148

Benzo[ghi]peryl	ne	
	+ acetophenone	153
	+ cyclohexane	150
	+ cyclohexanone	152
	+ ethyl butyrate	151
	+ heptane	150
	+ methylbenzene	151
	+ 2-propanone	152
Benzo[a]pyrene		
	+ benzene	155
	+ heptane	155
Biphenyl		
•	+ benzene	174-176
	+ benzophenone	194
	+ carbon disulfide	195
	+ chlorobenzene	190
	+ cyclohexane	167-170
	+ decahydronaphthalene	173
	+ 1,2-dibromoethane	188
	+ 1,4-dichlorobenzene	190, 191
	+ 1,1-dichloroethane	189
	+ 1,2-dichloroethane	189
	+ dichloromethane	184
	+ cis-1,2-dimethylcyclohexa	ne 171
	+ trans-1,2-dimethylcyclohe	xane 171
	+ cis-1,3-dimethylcyclohexa	ne 173
	+ cis-1,4-dimethylcyclohexa	ne 172
	+ trans-1,4-dimethylcyclohe	xane 172
	+ 2,6-dimethylnaphthalene	180
	+ 1,4-dioxane	182
	+ diphenylamine	199
	+ 1,2-diphenylethane	181
	+ diphenyl ether	183
	+ ethylbenzene	177
	+ heptane	159-163
	+ hexafluorobenzene	192
	+ hexane	158, 159
	+ indole	197, 198
	+ methylbenzene	177
	+ methylcyclohexane	170
	+ 2-methylnaphthalene	179
	+ naphthalene	178
	+ nitrobenzene	200
	+ octacosane	166
	+ 1-octadecanoic acid	201
	+ 1-octadecanol	193
	+ octane	163, 164
	+ 1-octanol	192
	+ pyridine	196
	+ tetrachloromethane	185-188
	+ tetracosane	165
	+ 1,2,3,4-tetrahydronaphtha	
	+ thiophene	196
	+ trichloromethane	184
a al mire est		
2,2'-Bipyridine	+ ethanol	204
	+ methanol	204
	+ 2-methyl-2-propanol + water	205 203 <b>–</b> 205
Buckminsterfull	rene + benzene	212 212
	+ benzene + benzonitrile	212, 213
		238
	+ hromohenzene	220 220
	<pre>+ bromobenzene + 1-bromo-2-methylnaphthale</pre>	229, 230 ne 236

Buckminsterfullerene		
1	butylbenzene	216
1	sec-butylbenzene t-butylbenzene	217 217
	carbon disulfide	237, 238
ì	chlorobenzene	230, 231
+	decane	210, 211
	1,2-dibromobenzene	231
	1,3-dibromobenzene	232
Į.	1,2-dibromoethane 1,2-dichlorobenzene	228
i e	1,3-dichlorobenzene	232, 233 233
	dichloromethane	225, 226
+	1,2-dimethylbenzene	218
1	1,3-dimethylbenzene	218
f .	1,4-dimethylbenzene	219 .
1	1,4-dioxane dodecane	224
	ethylbenzene	211 215
	fluorobenzene	235
+	hexane	209
+	2-hydroxymethylbenzene	237
	iodobenzene	236
3	methoxybenzene	225
1	methylbenzene 1-methylnaphthalene	213, 214
	2-methylthiophene	223, 224 241
1	nitrobenzene	239
+	octane	210
i	pentane	208
1	propylbenzene	215
1	iso-propylbenzene	216
l .	pyridine quinoline	239, 240
1	1,1,2,2-tetrachloroethane	240 229
1	tetrachloroethylene	228
	tetrachloromethane	227
+	1,2,3,4-tetramethylbenzene	222
	1,2,3,5-tetramethylbenzene	222
1	1,2,3,4-tetrahydronaphthalene tetrahydrothiophene	223
	thiophene	242 241
	1,2,4-trichlorobenzene	234
I .	trichloromethane	226
I .	1,2,3-trimethylbenzene	219
	1,2,4-trimethylbenzene	220
†	1,3,5-trimethylbenzene	221, 222
Carbazole		
1	acetic anhydride	281
1	acetophenone	277
1	benzene	256
l	1-butanol 2-butanone	272, 273
1	butyl butyrate	276
	t-butylcyclohexane	260 254
	carbon disulfide	277
I .	chlorocyclohexane	268
1	1-chlorohexane	267
1	1-chloroctane 1-chlorotetradecane	267
1	1-chiorotetradecane chrysene	268
	cyclohexane	258 249-251
	cyclohexanone	276
	cyclooctane	252
	decahydronaphthalene	255
	decane	247
†	dibenzofuran	285
<u> </u>		

Carbazole			
	+	1,4-dioxane	264
	+	N, N-dimethylacetamide	282
		1,4-dimethylbenzene	257
	+	N, N-dimethylformamide	283
	+	dimethyl sulfoxide	280
	+	dodecane	248
	+	1,2-ethanediol	271
	+	ethanol	269, 270
	+	ethyl ethanoate	259
	+	heptane	246
	+	hexadecane	248, 249
	+	hexane	245
	+	methanol	269
	+	methoxybenzene	264
	+	methylbenzene	257
	+	methylcyclohexane	251
	+	1-methyl-2-pyrrolidinone	282
		nitromethane	281
	+	octane	247
		1-octanol	273, 274
		1,1-oxybisbutane	262, 263
		1,1-oxybisethane	261, 262
		1,1-oxybisechane	263
		phenol	274
		1-propanol	271
		2-propanol	272
		<del>-</del> -	=
		2-propanone	275
		pyridine	278, 279
		quinoline	279
	+	2,6,10,15,19,23-hexamethyltetracosane	
			254
		tetrachloromethane	266
		tetrahydrofuran	261
	+	1,2,3,4-tetrahydronaphthalene	259
	+	tetrahydropyran	260
	+	tetramethylene sulfone	283
	+	thiophene	280
	+	tributyl phosphate	284
	+	trichloromethane	265, 266
	+	2,2,4-trimethylpentane	252, 253
Chrysene			
Curlence	_	acenaphthene	292
		anthracene	
			289
		benz[a]anthracene	290, 291
		benzene	287
		carbazole	297
		dibenzofuran	298
		fluoranthene	294
		fluorene	293
		heptane	287
	+	• • • • • • • • • • • • • • • • • • • •	288
	+	1-octanol	296
	+	pyrene	295
Coronene			
= =	+	heptane	300
	+	1-octanol	300
Dibenz[a,h]anth	races	•	
Procusta, mlanch			302
	+	heptane 1-octanol	302 302
			- <del></del>
Dibenzofuran	+	henzene	305 306
Dibenzofuran		benzene	305, 306
Dibenzofuran		cyclohexane	305, 306 304 304

Dibenzofuran		
+	pyridine	307
+	1,2,3,4-tetrahydronaphthalene	306
+	thiophene	307
Dibenzothiophene		
+	benzene	310, 311
+	cyclohexane	309
+	decahydronaphthalene	309
+	pyridine	312
+	1,2,3,4-tetrahydronaphthalene	311
+	thiophene	312
1,2-Diphenylbenzene		
+	benzene	314
+	cyclohexane	314
+	tetrachloromethane	315
1,3-Diphenylbenzene		
+	benzene	317
+	cyclohexane	317
+	tetrachloromethane	318
1,4-Diphenylbenzene		
+	benzene	320

# 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.

50-32-8	155
53-70-3	302
56-23-5	17, 55, 56, 185-188, 227, 266, 315, 318
56-55-3	146, 290, 291
57-11-4	201
60-29-7	50, 261, 262
62-53-3	76
64-17-5	18, 204, 269, 270
67-56-1	18, 60, 61, 142, 203, 269
67-63-0	63, 92-98, 136, 138, 139, 143, 272
67-64-1	69, 70, 152, 275
67-66-3	17, 54, 55, 184, 226, 265, 266
67-68-5	73, 74, 144, 280
68-12-2	80, 283
71-23-8	19, 62, 85-91, 134-137, 271
71-36-3	63, 64, 99-105, 134, 138, 272-274
71-43-2	4, 24, 37-41, 155, 174-176, 212, 213,
	256, 305, 306, 310, 311, 314, 317, 320
74-88-4	56
75-05-8	71, 141
75-09-2	184, 225, 226
75-15-0	72, 195, 237, 238, 277
75-34-3	189
75-52-5	281
75-65-0	205
78-83-1	65, 113-119
78-93-3	71, 276
79-01-6	58
79-34-5	229
83-32-9	2-21, 44, 292
84-15-1	314, 315
85-01-8	13
86-73-7	14, 293
86-74-8	245-285, 297
88-89-1	83

90-12-0	223, 224
91-17-8	3, 23, 37, 173, 255, 304, 309
91-20-3	8, 178, 288
91-22-5	78, 240, 279
91-57-6	9, 179
92-06-8	317, 318
92-52-4	158-201
92-94-4	320
95-47-6	6, 218
95-48-7	69, 237 ·
95-50-1	232, 233
95-63-6	220
95-93-2	7
98-06-6	217
98-82-8	216
98-86-2	153, 277
98-95-3	74, 75, 200, 239
99-87-6	43
100-41-4	177, 215
100-47-0	238
100-66-3	79, 225, 264
101-84-8	183
103-29-7	181
103-65-1	215
104-51-8	216
105-54-4	151
106-42-3	42, 43, 219, 257
106-46-7	190, 191
106-93-4	188, 228
107-06-2	189
107-21-1	271
108-24-7	73, 281
108-36-1	232
108-38-3	218
108-67-8	220, 221
108-86-1	59, 229, 230
108-87-2	34, 89, 96, 103, 110, 117, 124, 131,
	170, 251
108-88-3	5, 41, 42, 151, 177, 213, 214, 257
108-90-7	59, 60, 190, 230, 231
108-94-1	152, 276
108-95-2	68, 274

109-21-7	260
109-66-0	208
109-69-3	57
109-99-9	52, 261
110-01-0	78, 242
110-02-1	20, 26, 196, 241, 280, 307, 312
110-54-3	29, 85, 92, 99, 106, 113, 120, 127,
	158, 159, 209, 245
110-56-5	57
110-82-7	2, 3, 23, 32, 33, 88, 95, 102, 109,
	116, 123, 130, 150, 167-170, 249-251,
	304, 309, 314, 317
110-86-1	20, 26, 76, 77, 196, 239, 240, 278,
	279, 307, 312
111-01-3	36, 254
111-65-9	31, 87, 94, 101, 108, 115, 122, 129,
	163, 164, 210, 247
111-85-3	267
111-87-5	19, 66-68, 127-133, 137, 140, 148, 192,
	296, 300, 302
112-40-3	211, 248
112-92-5	193
119-61-9	194
119-64-2	5, 24, 47, 182, 223, 259, 306, 311
120-12-7	12, 29-144, 289
120-17-7	79
120-72-9	197, 198
120-82-1	234
122-39-4	199
123-51-3	65, 120-126
123-86-4	48
123-91-1	53, 54, 182, 224, 264
124-18-5	210, 211
126-33-0	81, 283
126-73-8	81, 284
127-18-4	228
127-19-5	80, 282
129-00-0	295
132-64-9	285, 298, 304-307
132-65-0	309~312
135-98-8	217
141-28-6	49

141-78-6	47, 259
142-18-5	247
142-68-7	52, 260
142-82-5	30, 86, 93, 100, 107, 114, 121, 128,
	146, 150, 155, 159-163, 246, 287, 300,
	302
142-96-1	50, 51, 262, 263
191-07-1	300
191-24-2	150-153
206-44-0	16, 46, 294
218-01-9	15, 45, 258, 287-298
243-17-4	147
260-94-6	23-25
292-64-8	34, 252
392-56-3	192
462-06-6	235
488-23-3	222
526-73-8	219
527-53-7	222
540-84-1	35, 84, 90, 97, 104, 111, 118, 125,
	132, 252, 253, 273, 274
541-73-1	233
542-18-7	268
544-10-5	267
544-76-3	31, 248, 249
554-14-3	241
581-42-0	10, 180
582-16-1	11
583-53-9	231
591-50-4	58, 236
593-45-3	2, 32
624-29-3	172
627-93-0	48
630-02-4	166
638-04-0	173
646-31-1	165
693-65-2	263
872-50-4	79, 282
2050-60-4	49
2207-01-4	171
2207-04-7	172
2425-54-9	268

2586-62-1	236
3178-22-1	36, 84, 91, 98, 105, 112, 119, 126,
	133, 254
3698-53-1	21, 82
6876-23-9	171
7732-18-5	141-144, 203-205
15892-23-6	64, 106-112, 135, 139, 140
99685-96-8	208-242

## **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.

30, 146, 150, 155, 161, 287, 300, Abuin, E.B. 302 xvi, xix, xxi, xxvi, xxxi, xxxii, Acree, W.E., Jr. xxxiv, xxxvii, 29-32, 34-37, 41, 42, 47-53, 55, 57, 62-65, 67, 84-140, 158, 159, 161-164, 167, 170, 185, 187, 188, 245-249, 251, 252, 254, 260, 262, 267, 268 Adjei, A. xxv 52, 53, 70, 71, 73, 77-81, 259, 261, Aleksandrov, V.V. 264, 270, 271, 275-277, 279-284 xxvii, 35, 51, 63, 66, 253, 260, Anderson, B.D. 263, 266, 272, 273, 278 Arnett, E.M. xxvi xxxvii, 3, 5, 23-25, 33, 37, 39, 47, Auwaerter, J.E. 76, 78, 173, 182, 251, 255, 256, 259, 278, 280, 304, 306, 307, 309, 311, 312 Barton, A.F.M. xxiii xxv Beerbower, A. Belloto, R.J., Jr. xxvi Berchiesi, G. 193, 201 Bertrand, G.L. xxvi Bissell, M. 52, 53 Brandts Buys, X.M. xxviii Braton, C.M. xxi Brennecke, J.F. 150-153 Buchmann, M. xxviii-xxx Buchowski, H. xxxvii Buehring, K.G. 3, 4, 167, 174 Burgess, J. 203-205 Carre, O.R. 150-153 Chang, W. xxiv, 158, 163, 164, 168, 170-174, 177, 184, 185, 188-190, 195 Chernyi, A.V. 52, 53, 70, 71, 73, 77-81, 259, 261, 264, 270, 271, 275-277, 279-284 Chickos, J.S. xxi Chiou, C.T. xxii Chittick, C.E. 52, 53 Choi, P.B. xviii, 3, 4, 20, 167, 174, 196 Christian, S.D. xxvii Cline, P.V. 54, 58, 60, 61, 67, 69, 71, 74, 75, 141-144 Cook, W.A. 191 xxxvii, 3, 5, 23-25, 33, 37, 39, 47, Coon, J.E. 76, 78, 173, 182, 251, 255, 256, 259, 278, 280, 304, 306, 307, 309,

311, 312

Cordero, Y.	48, 49
Cullinane, N.M.	285
Dhamodaran, R.	208-213, 220, 224, 225, 227, 237
Dixon, W.B.	xxvii
Djordjevic, N.M.	2, 32
Doane, E.P.	72
Domanska, U.	xxxvii, 305, 310
Drickamer, H.G.	72
Duer, W.C.	xxvi
Ebina, T	197
Fletcher, A.H.	xxvii
Fohl, J.	38, 42, 43, 54, 56, 60, 68, 69, 72,
	77, 250, 256, 257, 265, 266, 269,
	272, 274, 275, 277
Fris, M.	38, 42, 43, 54, 56, 60, 68, 69, 72,
,	77, 250, 256, 257, 265, 266, 269,
	272, 274, 275, 277
Fuchs, F.H.	xxvi
Fuchs, R.	xxvi
Fung, HL.	245-250, 253, 262, 265
Gomes de Azevedo, E.	xvii
Gordon, L.J.	xxx
Gorrie, T.M.	xxvi
Grant, D.J.W.	xvi
Groves, F.R., Jr.	305, 310
Gupta, P.D.	75, 200
Haines, R.I.	203-205
Halmi, J.L.	41
Haulait-Pirson, M.C.	xxviii
Heller, C.A.	xxvii
Hesse, D.G.	xxi
Higuchi, T.	xvi, xxvii, 245-250, 253, 262, 265
Hildebrand, J.H.	xvii
Hofman, T.	xxxvii
Hollinger, H.B.	xxvii
Hoy, K.L.	xxiii
Huang, GL.	19, 66, 148, 192, 296, 300, 302
Huyskens, P.L.	xxviii
James, K.C.	xvii
Joris, L.	xxvi
Judy, C.L.	159, 161, 164, 170, 188
Kaliappan, I.	208-213, 220, 224, 225, 227, 237
Kesselring, V.W.	xxviii-xxx, 270, 271, 273, 274
Kohli, D.	xxvi
Kravchenko, V.M.	6-16, 44-46, 258, 288, 289, 291-295,
	297, 298
Lawe, T.	290
Lee, H.H.	178, 181, 194, 199
Lee, L.S.	54, 58, 60, 61, 67, 69, 71, 74, 75,
	141-144
Lichtenthaler, R.N.	xvii
Liebman, J.F.	xxi
Lissi, E.A.	30, 146, 150, 155, 161, 287, 300,
	302
Lorents, D.C.	208, 209, 211, 212, 214, 221, 223,
	225-230, 232, 234, 235, 237-239,
	241, 242

19, 66, 148, 192, 296, 300, 302 Mackay, D. 29, 33, 39, 50, 55, 59, 61, 62, 70, Mahieu, J. 74, 76 208, 209, 211, 212, 214, 221, 223, Malhotra, R. 225-230, 232, 234, 235, 237-239, 241, 242 xxii Manes, M. 50 Marthandan, M.V. xxv Martin, A. 62, 64, 85-90, 99-104 Martinez, E. 208-213, 220, 224, 225, 227, 237 Mathews, C.K. xxvi, xxxi, xxxvii, 31, 36, 51, 245-McCargar, J.W. 249, 251, 252, 254, 260, 262, 267, 268 xxvii McClellan, M.L. xviii, xxxvii, 2-5, 17, 20, 23-25, McLaughlin, E. 33, 37, 39, 41, 47, 76, 78, 167, 168, 173-175, 182, 186, 192, 196, 251, 255, 256, 259, 278, 280, 287, 304-307, 309-312, 314, 315, 317, 318, 320 192 Messer, C.E. Miller, M.M. 19, 66, 148, 192, 296, 300, 302 Mishra, D.S. Mitchell, E. xxvi 191 Morris, R.E. 41 Murral, D.J. xxvi Murty, T.S.S.R. xxviii-xxx Nam-Tran, H. 52, 53, 70, 71, 73, 77-81, 259, 261, Nazarov, V.N. 264, 270, 271, 275-277, 279-284 Newburger, J. xxv Ochsner, A.B. xxvi 41 Oswalt, B.M. 38, 56, 58 Palit, S.R. 6-16, 44-46, 258, 288, 289, 291-295, Pastukhova, I.S. 297, 298 Pemenzi, D. xix Phillips, D.J. 150-153 Pimental, G.C. xxvii Pinal, R. 54, 58, 60, 61, 67, 69, 71, 74, 75, 141-144 Pontikos, N.M. 159, 161, 164, 170, 188 Prausnitz, J.M. xvii, xviii, xxv Procyk, A.D. Rao, P.S.C. 54, 58, 60, 61, 67, 69, 71, 74, 75, 141-144 Rees, W.T. 285 Rey-Mermet, C. xxviii-xxx Richtol, H.H. xxvii Rodewald, R.F. xxvi Rubstov, V.I. 52, 53, 70, 71, 73 , 77-81, 259, 261, 264, 270, 271, 275-277, 279-284 Ruelle, P. xxviii-xxx, 270, 271, 273, 274 208, 209, 211, 212, 214, 221, 223, Ruoff, R.S. 225-230, 232, 234, 235, 237-239, 241, 242

xxvii, xxxii, 29-32, 34, 35, 37 Rytting, J.H. xix Sabbah, R. Saluja, P.P.S. xxvi xxviii-xxx, 270, 271, 273, 274 Sarraf, E. 160, 175, 182, 186, 190, 195 Scheib, R.C. Schleyer, P.v.R. xxvi xvii, xxx Scott, R.L. 213-222, 224, 230-236, 240, 241 Scrivens, W.A. xxxvii, 23-25, 33, 39, 76, 78, 251, Sediawan, W.B. 256, 278, 280, 304, 306, 307, 309, 311, 312 xvii Shinoda, K. 21, 82 Shinomiya, C. 19, 66, 148, 192, 296, 300, 302 Shiu, W.-Y. Shukla, B.M. Siegel, G.G. xxviii Singh, N.P. 83 208-213, 220, 224, 225, 227, 237 Sivaraman, N. Smith, B. 48, 49 38, 42, 43, 54, 56, 60, 68, 69, 72, Smutek, M. 77, 250, 256, 257, 265, 266, 269, 272, 274, 275, 277 Sokoloski, T.D. xxvi 38, 56, 58 Somayajulu, G.R. Speyers, C.L. 5, 17-19 208-213, 220, 224, 225, 227, 237 Srinivasan, R.G. 75, 200 Srivastava, R.D. 53 Street, K.W., Jr. Sturrock, M.G. 290 160, 175, 182, 186, 190, 195 Svirbely, W.J. Szafranski, A.M. 179, 180, 183, 198 197 Takahashi, S. xxvi, xxxvii, 62, 64, 85-90, 99-104, Teng, I.-L. 260, 262 213-222, 224, 230-236, 240, 241 Tour, J.M. 62, 64, 85-90, 99-104 Trejo, J. 208, 209, 211, 212, 214, 221, 223, Tse, D.S. 225-230, 232, 234, 235, 237-239, 241, 242 xxvii Tucker, E.E. 34, 41, 42, 55, 63, 67, 92-97, 127-Tucker, S.A. 132 52, 53, 70, 71, 73, 77-81, 259, 261, Vail, E.I. 264, 270, 271, 275-277, 279-284 Valvani, S.C. хx van der Borght, X. xxviii Vanderheyden, G. xxviii Van Ness, H.C. xxvii Van Winkle, J. xxvii 208-213, 220, 224, 225, 227, 237 Vasudeva Rao, P.R. Vitali, G. 165, 166 160, 175, 178, 181, 182, 186, 190, Warner, J.C. 194, 195, 199 19, 66, 148, 192, 296, 300, 302 Wasik, S.P. Weimer, R.F. xviii Wheeler, A.S. 43 Williams, C.P. 3, 4, 167, 174

Wolfe, J.

Wu, P.L.

Wyrzykowska-Stankiewicz, D.

Yalkowsky, S.H.

Yokoyama, C.

Young, T.M.

Zainal, H.A.

Zvaigzne, A.I.

65, 113-119

xxv

179, 180, 183, 198

xx, 54, 58, 60, 61, 67, 69, 71, 74,

75, 141-144, 155

197

xxvi

2, 4, 17, 41, 168, 175, 186, 287,

314, 315, 317, 318, 320

xxvi, xxxiv, xxxvii, 36, 47-49, 57,

62-65, 67, 84-140, 260, 262

# **SOLUBILITY DATA SERIES**

Volume 1	H. L. Clever, Helium and Neon
Volume 2	H. L. Clever, Krypton, Xenon and Radon
Volume 3	M. Salomon, Silver Azide, Cyanide, Cyanamides, Cyanate,
V 3133310 0	Selenocyanate and Thyocyanate
Volume 4	H. L. Clever, Argon
Volume 5/6	C. L. Young, Hydrogen and Deuterium
Volume 7	R. Battino, Oxygen and Ozone
Volume 8	C. L. Young, Oxides of Nitrogen
Volume 9	W. Hayduk, Ethane
Volume 10	R. Battino, Nitrogen and Air
Volume 11	B. Scrosati and C. A. Vincent, Alkali Metal, Alkaline Earth Metal and
	Ammonium Halides, Amide Solvents
Volume 12	C. L. Young, Sulfur Dioxide, Chlorine, Fluorine and Chlorine Oxides
Volume 13	S. Siekierski, T. Mioduski and M. Salomon, Scandium, Yttrium,
	Lanthanum and Lanthanide Nitrates
Volume 14	H. Miyamoto, M. Salomon and H. L. Clever, Alkaline Earth Metal
	Halates
Volume 15	A. F. M. Barton, Alcohols with Water
Volume 16/17	E. Tomlinson and A. Regosz, Antibiotics: 1, β-Lactam Antiobiotics
Volume 18	O. Popovych, Tetraphenylborates
Volume 19	C. L. Young, Cumulative Index: Volumes 1-18
Volume 20	A. L. Horvath and F. W. Getzen, Halogenated Benzenes, Toluenes and
	Phenols with Water
Volume 21	C. L. Young and P. G. T. Fogg, Ammonia, Amines, Phosphine, Arsine,
37-1 - 00	Stibine, Silane, Germane and Stannane in Organic Solvents
Volume 22	T. Mioduski and M. Salomon, Scandium, Yttrium, Lanthanum and
Volume 23	Lanthanide Halides in Nonaqueous Solvents T. P. Ditkse, Copper, Silver, Gold and Zinc, Cadmium, Mercury Oxides
Volume 25	and Hydroxides
Volume 24	W. Hayduk, Propane, Butane and 2-Methylpropane
Volume 25	C. Hirayama, Z. Galus and C. Guminski, Metals in Mercury
Volume 26	M. R. Masson, H. D. Lutz and B. Engelen, Sulfites, Selenites and
Volume 20	Tellurites
Volume 27/28	H. L. Clever and C. L. Young, Methane
Volume 29	H. L. Clever, Mercury in Liquids, Compressed Gases, Molten Salts and
Volume 27	Other Elements
Volume 30	H. Miyamoto and M. Salomon, Alkali Metal Halates, Ammonium Iodate
VOIDENC 30	and Iodic Acid
Volume 31	J. Eysseltová and T. P. Dirske, Alkali Metal Orthophosphates
Volume 32	P. G. T. Fogg and C. L. Young, Hydrogen Sulfide, Deuterium Sulfide and
V 0101110 02	Hydrogen Selenide
Volume 33	P. Franzosini, Molten Alkali Metal Alkanoates
Volume 34	A. N. Paruta and R. Piekos, 4-Aminobenzenesulfonamides.
·	Part I: Non-cyclic Substitutents
Volume 35	A. N. Paruta and R. Pickos, 4-Aminobenzenesulfonamides.
·	Part II: 5-Membered Heterocyclic Substituents

Volume 36	A. N. Paruta and R. Pickos, 4-Aminobenzenesulfonamides.  Part III: 6-Membered Heterocyclic Substituents and Miscellaneous  Systems
Volume 37	D. G. Shaw, Hydrocarbons with Water and Seawater.  Part I: Hydrocarbons $C_5$ to $C_7$
Volume 38	D. G. Shaw, Hydrocarbons $C_5$ to $C_7$ Part II: Hydrocarbons $C_8$ to $C_{36}$
Volume 39	C. L. Young, Cumulative Index: Volumes 20–38
Volume 40	J. Hala, Halides, Oxyhalides and Salts of Halogen Complexes of
	Titanium, Zirconium, Hafnium, Vanadium, Niobium and Tantalum
Volume 41	CY. Chan, I. N. Lepeshkov and K. H. Khoo, Alkaline Earth Metal
	Perchlorates
Volume 42	P. G. T. Fogg and W. Gerrard, Hydrogen Halides in Non-aqueous
	Solvents
Volume 43	R. W. Cargill, Carbon Monoxide
Volume 44	H. Miyamoto, E. M. Woolley and M. Salomon, Copper and Silver
	Halates
Volume 45/46	R. P. T. Tomkins and N. P. Bansal, Gases in Molten Salts
Volume 47	R. Cohen-Adad and J. W. Lorimer, Alkali Metal and Ammonium
	Chlorides in Water and Heavy Water (Binary Systems)
Volume 48	F. Getzen, G. Hester and A. Maczynski, Esters with Water.
	Part 1: Esters 2-C to 6-C
Volume 49	F. Getzen, G. Hester and A. Maczynski, Esters with Water.
	Part II: Esters 7-C to 32-C
Volume 50	P. G. T. Fogg, Carbon Dioxide in Non-aqueous Solvents at Pressures
	Less Than 200 kPa
Volume 51	J. G. Osteryoung, M. M. Schreiner, C. Guminski and Z. Galus,
	Intermetallic Compounds in Mercury
Volume 52	I. Lambert and H. L. Clever, Alkaline Earth Hydroxides in Water and
	Aqueous Solutions
Volume 53	C. L. Young, Cumulative Index: Volumes 40-52
Volume 54	W. E. Acree, Jr, Polycyclic Aromatic Hydrocarbons in Pure and Binary
	Solvents
Volume 55	S. Siekierski and S. L. Phillips, Actinide Nitrates
Volume 56	D. Shaw, A. Skrzecz, J. W. Lorimer and A. Maczynski, Alcohols with
	Hydrocarbons
Volume 57	W. Hayduk, Ethene