IUPAC-NIST Solubility Data Series. 98. Solubility of Polycyclic Aromatic Hydrocarbons in Pure and Organic Solvent Mixtures—Revised and Updated. Part 3. Neat Organic Solvents

William E. Acree, Jr.[a)]

Department of Chemistry, University of North Texas, Denton, Texas 76203, USA

(Received 28 November 2012; accepted 30 November 2012; published online 4 March 2013)

This work updates Vols. 54, 58, and 59 in the IUPAC Solubility Data Series and presents solubility data for polycyclic aromatic hydrocarbon solutes dissolved in neat organic solvents. Published solubility data for acenaphthene, anthracene, biphenyl, carbazole, dibenzofuran, dibenzothiophene, fluoranthene, fluorene, naphthalene, phenanthrene, phenothiazine, pyrene, thianthrene, and xanthene that appeared in the primary literature from 1995 to the end of 2011 are compiled and critically evaluated. Experimental solubility data for more than 550 different solute-organic solvent systems are included. Solubility data published prior to 1995 were contained in three earlier volumes (Vols. 54, 58, and 59) and are not repeated in this volume. © *2013 American Institute of Physics.* [http://dx.doi.org/10.1063/1.4775402]

Key words: acenaphthene; alcohols; alkanes; alkanenitriles; alkoxyalcohols; alkyl ethanoates; anthracene; biphenyl; carbazole; chloroalkanes; dialkyl ethers; dibenzofuran; dibeznothiophene; fluoranthene; fluorine; naphthalene; phenanthrene; phenothiazine; polycyclic aromatic hydrocarbons; pyrene; solubility; thainthrene; xanthenes.

CONTENTS

[a)] Electronic mail: acree@unt.edu.

List of Tables

1. Preface

1.1. Scope of this volume

Volumes 54,[1] 58,[2] and 59 (Ref. 3) in the IUPAC Solubility Data Series dealt with the solubility of polycyclic aromatic hydrocarbons (PAHs) and polycyclic aromatic hetero-atom compounds (PAHaCs) in both neat organic solvents and binary organic solvents. The specific solutes considered included: acenaphthene, acridine, anthracene, benz[a]anthracene, benzo[b]fluorene, benzo[ghi]perylene, benzo[a]pyrene, biphenyl, 2,2′-bipyridine, buckminsterfullerene (C60), carbazole, chrysene, coronene, dibenz[a,h]anthracene, dibenzofuran, dibenzothiophene, 1,2-diphenylbenzene, 1,3-diphenylbenzene, 1,4-diphenylbenzene, fluoranthene, fluorene, indole, naphthacene, naphthalene, perylene, phenanthrene, 1,10-phenanthroline, phenothiazine, phenoxanthiin, phenoxazine, pyrene, thianthrene, thioxanthene, triphenylene, and xanthenes. The three volumes covered the published literature up to 1995, including several articles that were still in press at the time.

This is the last part of the three-part series that updates the three earlier volumes on PAH and PAHaC solubilities. Part 1 (Ref. 4) was devoted to solubilities in binary solvent mixtures, and incorporates compilations based on papers published in the peer-reviewed scientific literature between 1995 to the end of 2011. Part 2 (Ref. 5) dealt with solubilities of PAHs and PAHaCs dissolved in ternary solvent mixtures. Part 3 (the present paper) will focus on the organic mono-solvents (neat organic solvents). To conserve space, data from the earlier volumes will not be repeated here.

1.2. Procedures used in critical evaluation of published solubility data

The different concentration units that are used to express experimental solubility data, and the thermodynamic principles that govern solubility solid-liquid equilibria, were described in Part 1 of this volume.[4] The only part of the earlier discussion that will be repeated here pertains to the mathematical representation of solubility data for crystalline nonelectrolyte solutes as a function of temperature.

Published solubility data may be found for a given solute-solvent system measured at several different temperatures. The temperature variation can be critically evaluated using standard thermodynamic relationships based on the ideal mole fraction solubility of a solid solute, ${x_1}^{\text{ideal soly}}$ in a liquid solvent[6]

$$-\ln {x_1}^{\text{ideal soly}} = \frac{\Delta {H_1}^{\text{fus}}}{RT}\left[1-\frac{T}{T_{\text{mp}}}\right] + \frac{\Delta C_{p,1}}{R}\left(\frac{T_{\text{mp}}-T}{T}\right) + \frac{\Delta C_{p,1}}{R}\ln\left(\frac{T_{\text{mp}}}{T}\right), \tag{1}$$

where $\Delta {H_1}^{\text{fus}}$ is the standard molar enthalpy of fusion of the solute at its normal melting point temperature, T_{mp}, $\Delta C_{p,1}$ is the difference in the molar heat capacities of the liquid and crystalline forms of the solute (i.e., $\Delta C_{p,1} = C_{p,\text{liquid}} - C_{p,\text{solid}}$) and R is the universal gas constant. Through suitable algebraic manipulations, Eq. (1) can be rearranged to give

$$\ln {x_1}^{\text{ideal soly}} = \left[\frac{\Delta {H_1}^{\text{fus}}}{R\,T_{\text{mp}}} + \frac{\Delta C_{p,1}}{R}\,(1+\ln T_{\text{mp}})\right] - \left(\frac{\Delta {H_1}^{\text{fus}}}{R} + \frac{\Delta C_{p,1} T_{\text{mp}}}{R}\right)\frac{1}{T} + \frac{\Delta C_{p,1}}{R}\ln T, \tag{2}$$

which has the generalized mathematical form of

$$\ln x_1 = A + \frac{B}{T} + C\ln T. \tag{3}$$

Though derived for an ideal solution, Eq. (3) has been used successfully to describe solute solubility in many nonideal solutions. The equation is commonly referred to as the Modified Apelblat equation in the literature.

The λh model, developed by Buchowski *et al.*,[7,8] is

$$\ln\left[1+\frac{\lambda(1-x_1)}{x_1}\right]=\lambda h\left(\frac{1}{T}-\frac{1}{T_{\mathrm{mp}}}\right), \qquad (4)$$

a second popular mathematical representation for describing how the mole fraction solubility varies with solution temperature. In Eq. (4), T and T_{mp} refer to the solution temperature and melting point temperature of the solute, respectively. The two model parameters, λ and h, are determined by least-squares analyses using the measured mole fraction solubilities. Experimental solubility data are considered to be internally consistent if the measured x_1 values can be accurately described by either Eq. (3) and/or Eq. (4).

2. Solubility of Acenaphthene in Organic Solvents

2.1. Critical evaluation of experimental solubility data

Volume 58 in the IUPAC Solubility Data Series[2] contained experimental solubility data for acenaphthene in three saturated hydrocarbons (octadecane, cyclohexane and decahydronaphthene), in four aromatic hydrocarbons (benzene, methylbenzene, 1,2-dimethylbenzene, and 1,2,3,4-tetrahydronaphthalene), in two haloalkanes (trichloromethane and tetrachloromethane), in four alkanols (methanol, ethanol, 1-propanol, and 1-octanol) and in two miscellaneous organic solvents (pyridine and thiophene). The majority of systems included measurements at several temperatures covering a 30 to 40 K range. The compiled solubility data also included phase diagram information for binary 1,2,4,5-tetramethylbenzene + acenaphthene, naphthalene + acenaphthene, 2-methylnaphthalene + acenaphthene, 2,6-dimethylnaphthalene + acenaphthene, 2,7-dimethylnaphthalene + acenaphthene, anthracene + acenaphthene, phenanthrene + acenaphthene, fluorene + acenaphthene, chrysene + acenaphthene, fluoranthene + acenaphthene and 1,2,3,5-tetranitrobenzene + acenaphthene mixtures. Solubility data contained in Vol. 58 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for acenaphthene.

There have been several studies that reported solubility data for acenaphthene dissolved in organic solvents after Vol. 58 was published in 1995. De Fina *et al.*[9] determined the solubility of acenaphthene in 36 different organic solvents containing ether-, carbonyl-, hydroxy-, ester-, methyl-, and *tert*-butyl functional groups. The experimental measurements were performed at the single temperature of 298.15 K and used to test the limitations and applications of predictive expressions based on Mobile Order theory. Acree and Abraham[10] measured acenaphthene solubilities at 298.15 K in 11 additional solvents, namely, squalane, 2-methoxy-2-methylpropane (more commonly called methyl *tert*-butyl ether), 1,1′-oxybisethane (also called diethyl ether), 2,2′-oxybispropane (also called diisopropyl ether), 3,7-dimethyl-1-octanol, butanone, methyl ethanoate, propanenitrile, butanenitrile, dimethyl sulfoxide, and *N*-methylformamide. For the majority of the solvents studied by De Fina *et al.*[9] and by Acree and Abraham[10] there is only the single experimental value, and it is not possible to perform a critical evaluation on most of the published data.

There does exist independent solubility data for acenaphthene in cyclohexane in Vol. 58 of the Solubility Data Series[2] at temperatures slightly greater than 298.15 K. McLaughlin and Zainal[11] conducted acenaphthene solubility measurements from 308.7 to 334.0 K. Choi *et al.*[12] subsequently determined the solubility at 303.4–354.5 K. There is approximately a 10%–15% relative deviation between the two independent sets of measurements. Analysis of the two datasets using Eq. (3) with $C=0$ gave the following two mathematical correlations:

$$\ln x_1 = 15.534-\frac{5541.3}{T}, \qquad (5)$$

$$\ln x_1 = 13.202-\frac{4757.9}{T}. \qquad (6)$$

The calculated equation coefficients reflect the differences in the two datasets. Equations (5) and (6) provide a reasonably accurate mathematical description of the experimental mole fraction solubilities in the respective dataset. Differences between the experimental data and values back-calculated using Eqs. (5) and (6) were on the order of 3.6% or less. Equations (5) and (6) give extrapolated values of $x_1 = 0.04726$ and $x_1 = 0.006356$ for the mole fraction solubility of acenaphthene in cyclohexane at 298.15 K, which are both less than the value of $x_1 = 0.07043$ that was reported by De Fina *et al.*[9] Differences in chemical purities and experimental methodologies were the likely causes of the deviations noted in the published solubility data for acenaphthene dissolved in cyclohexane.

Two groups have studied the solubility of acenaphthene as a function of temperature. Kotula and Marciniak[13] published solubility data for acenaphthene in four chlorinated alkanes (trichloromethane, tetrachloromethane, 1,1-dichloroethane, and 1,2-dichloroethane) and two chlorinated alkenes (trichloroethene and tetrachloroethene) from 290 to 325 K. He and Liu[14] employed a synthetic method to measure the solubility of acenaphthene in ethanol, 2-propanol, 1-butanol, and methylbenzene at ten different temperatures covering the range of 278–323 K. The experimental values determined by He and Liu[14] for acenaphthene in ethanol ($x_1 = 0.01079$), 2-propanol ($x_1 = 0.01197$), and 1-butanol ($x_1 = 0.02367$) differ by an average deviation of less than 5% from the measured values of De Fina *et al.*[9] (ethanol, $x_1 = 0.01068$; 2-propanol, $x_1 = 0.01336$; and 1-butanol, $x_1 = 0.02373$). Deviations of this magnitude are often attributed to differences in chemical purities and experimental methodologies.

TABLE 1. Parameters of the Apelblat equation for describing the solubility of acenaphthene in various organic solvents

Solvent	*A*	*B*	*C*	MRD (%)
Trichloromethane	7.354	−2690.2	0	0.1
Tetrachloromethane	8.311	−3041.8	0	0.7
1,1-Dichloroethane	8.086	−2959.3	0	0.4
1,2-Dichloroethane	7.871	−2885.7	0	0.1
Trichloroethene	7.480	−2743.4	0	0.6
Tetrachloroethene	8.454	−3099.4	0	0.1
Methylbenzene[a]	−53.186	21.255	9.033	0.3
Ethanol[a]	−73.395	−83.508	12.137	0.7
2-Propanol[a]	−71.517	−512.22	12.081	0.7
1-Butanol[a]	−93.112	844.83	15.186	0.7

[a] Numerical values of the coefficients and the percent mean relative deviations were taken from He and Liu.[14]

The internal consistency of the chloroalkane and chloroalkene datasets of measured acenaphthene solubilities, as well as the He and Liu[14] dataset, were assessed by curve-fitting the measured mole fraction solubility data to Eq. (3). The numerical values of the equation coefficients (*A*, *B*, and *C*) are given in Table 1, along with the mean relative deviation (MRD) calculated according to Eq. (7)

$$\text{MRD} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{x_1^{\text{exp}} - x_1^{\text{calc}}}{x_1^{\text{exp}}}\right|, \qquad (7)$$

where N is the number of experimental solubility measurements in an individual solute-solvent data set. Examination of the numerical entries in the last column of Table 1 reveals that the largest mean relative percent deviation between the back-calculated values based on Eq. (3) and experimental data is only 0.7%,which is less than the experimental uncertainties in the measured values. Results of the mathematical representation analyses indicate that the experimental data for all ten acenaphthene-organic solvent systems are internally consistent.

The experimental solubility data for acenaphthene dissolved in the different organic solvents are in Secs. 2.2–2.10.

2.2. Acenaphthene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Hexane; C_6H_{14}; [110-54-3]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9481	0.05192

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Heptane; C_7H_{16}; [142-82-5]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9393	0.06075

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Octane; C_8H_{18}; [111-65-9]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$ [a]	x_2 [b]	x_1 [c]
1.0000	0.9317	0.06826

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Nonane; C_9H_{20}; [111-84-2]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$ [a]	x_2 [b]	x_1 [c]
1.0000	0.9279	0.07210

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Decane; $C_{10}H_{22}$; [124-18-5]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$ [a]	x_2 [b]	x_1 [c]
1.0000	0.9215	0.07852

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Undecane; $C_{11}H_{24}$; [1120-21-4]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9164	0.08355

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in undecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Dodecane; $C_{12}H_{26}$; [112-40-3]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9120	0.08799

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in dodecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8935	0.1065

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Hexatriacontane; $C_{36}H_{74}$; [630-06-8]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
350.30	1.0000	0.0000
348.89	0.8878	0.1122
348.56	0.8482	0.1518
347.70	0.7926	0.2074
346.21	0.6886	0.3114
345.35	0.5931	0.4069
344.75	0.5537	0.4463
343.53	0.4629	0.5371
348.56	0.3953	0.6047
350.88	0.3005	0.6995
353.63	0.2517	0.7483
356.88	0.2029	0.7971
359.50	0.1510	0.8490
362.12	0.1006	0.8994
365.35	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a sum of symmetrized functions (SSF) to describe the activity coefficients of acenaphthene and hexatricontane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 343.4$ and eutectic mole fraction of acenaphthene of $x_1 = 0.548$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) Pure Grade, Prolabo, no purification details were given in the paper.
(2) 98+%, Fluka Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9296	0.07043

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9191	0.08093

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9026	0.09739

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9533	0.04668

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9224	0.07763

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8572	0.1428

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

2.3. Acenaphthene solubility in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Methylbenzene; C_7H_8; [108-88-8]	[14]F. He and P. Liu, J. Chem. Eng. Data **52**, 2536 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
278.47	0.8958	0.1042
283.33	0.8782	0.1218
288.10	0.8582	0.1418
293.15	0.8330	0.1670
298.23	0.8064	0.1936
303.15	0.7761	0.2239
307.95	0.7441	0.2559
312.95	0.7015	0.2985
318.30	0.6543	0.3457
323.20	0.6016	0.3984

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

The authors refer to the compound has 1,8-dihydroacenaphthalene, which the compiler has taken to be acenaphthene.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

2.4. Acenaphthene solubility data in esters

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9290	0.07100

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8914	0.1086

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8630	0.1370

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.7%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

2.5. Acenaphthene solubility data in ethers

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8981	0.1019

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9149	0.08505

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8884	0.1116

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9081	0.0919

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8027	0.1973

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution;
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	**Original Measurements:** [9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8585	0.1415

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

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

Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.

(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

2.6. Acenaphthene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components: (1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Trichloromethane; $CHCl_3$; [67-66-3]	**Original Measurements:** [13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
289.25	0.8575	0.1425
293.55	0.8364	0.1636
300.45	0.7979	0.2021
305.25	0.7678	0.2322
313.65	0.7057	0.2943
316.05	0.6861	0.3139
319.45	0.6558	0.3442
321.45	0.6379	0.3621
324.05	0.6124	0.3876

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, electric glass furnace, heater, mercury thermometer.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute and solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of a stereoscopic microscope.

Source and Purity of Chemicals:

(1) Analytically pure, International Enzymes Limited, Windsor-Bershire, England, recrystallized twice from distilled benzene and then from anhydrous ethanol.

(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:

Temperature: ±0.3 K.

x_1: < 1% (relative error).

Components: (1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Tetrachloromethane; CCl_4; [56-23-5]	**Original Measurements:** [13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
291.15	0.8805	0.1195
298.85	0.8491	0.1509
302.65	0.8232	0.1768
306.65	0.8001	0.1999
310.15	0.7750	0.2250
316.95	0.7230	0.2770
321.15	0.6860	0.3140
327.15	0.6279	0.3721

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute and solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of a stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, International Enzymes Limited, Windsor-Bershire, England, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) Purity not given, Polish Chemical Reagents, Gliwice, Poland, was dried over anhydrous sodium sulfate and then fractionally distilled.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,1-Dichloroethane; $C_2H_4Cl_2$; [75-34-3]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.65	0.8853	0.1147
290.15	0.8795	0.1205
296.85	0.8479	0.1521
300.35	0.8292	0.1708
305.35	0.7978	0.2022
312.95	0.7469	0.2531
319.15	0.6962	0.3038
320.45	0.6805	0.3195
323.75	0.6528	0.3472

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute and solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of a stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, International Enzymes Limited, Windsor-Bershire, England, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) Purity not given, Polish Chemical Reagents, Glowice, Poland, was dried over anhydrous sodium sulfate and then fractionally distilled.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.15	0.8828	0.1172
290.85	0.8712	0.1288
297.15	0.8413	0.1587
298.15	0.8362	0.1638
304.65	0.7981	0.2019
314.45	0.7293	0.2707
321.35	0.6700	0.3300
323.25	0.6522	0.3478

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute and solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of a stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, International Enzymes Limited, Windsor-Bershire, England, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Trichloroethene; C_2HCl_3; [79-01-6]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
289.15	0.8658	0.1342
292.35	0.8510	0.1490
297.45	0.8248	0.1752
306.15	0.7728	0.2272
311.05	0.7380	0.2620
312.75	0.7254	0.2746
315.05	0.7069	0.2931
318.85	0.6752	0.3248
322.85	0.6384	0.3616

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, electric glass furnace, heater, mercury thermometer.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute and solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of a stereoscopic microscope.

Source and Purity of Chemicals:

(1) Analytically pure, International Enzymes Limited, Windsor-Bershire, England, recrystallized twice from distilled benzene and then from anhydrous ethanol.

(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:

Temperature: ±0.3 K.

x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Tetrachloroethene; C_2Cl_4; [127-18-4]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.15	0.9000	0.1000
292.45	0.8828	0.1172
297.65	0.8590	0.1410
301.25	0.8401	0.1599
306.75	0.8082	0.1918
311.75	0.7741	0.2259
314.25	0.7556	0.2444
319.85	0.7905	0.2905
322.15	0.6887	0.3113

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, electric glass furnace, heater, mercury thermometer.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute and solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of a stereoscopic microscope.

Source and Purity of Chemicals:

(1) Analytically pure, International Enzymes Limited, Windsor-Bershire, England, recrystallized twice from distilled benzene and then from anhydrous ethanol.

(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:

Temperature: ±0.3 K.

x_1: < 1% (relative error).

2.7. Acenaphthene solubility data in alcohols

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Methanol; CH_4O; [67-56-1]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9946	0.00544

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.

[b] x_2: mole fraction of component 2 in the saturated solution.

[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Ethanol; C_2H_6O; [64-17-5]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9893	0.01068

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Ethanol; C_2H_6O; [64-17-5]	[14]F. He and P. Liu, J. Chem. Eng. Data **52**, 2536 (2007).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.10	0.9954	0.004622
283.53	0.9942	0.005785
288.25	0.9929	0.007093
293.25	0.9911	0.008913
298.20	0.9892	0.010793
303.20	0.9867	0.013276
308.20	0.9835	0.016519
313.05	0.9803	0.019700
318.25	0.9755	0.024486
323.15	0.9704	0.029553

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors refer to the compound as 1,8-dihydroacenaphthalene, which the compiler has taken to be acenaphthene.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1-Propanol; C_3H_8O; [71-23-8]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9831	0.01686

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Propanol; C_3H_8O; [67-63-0]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9866	0.01336

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Propanol; C_3H_8O; [67-63-0]	[14]F. He and P. Liu, J. Chem. Eng. Data **52**, 2536 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.30	0.9953	0.004687
283.07	0.9941	0.005923
288.33	0.9923	0.007701
293.20	0.9903	0.009671
298.07	0.9880	0.011972
303.30	0.9848	0.015233
308.05	0.9811	0.018871
312.95	0.9764	0.023581
318.40	0.9698	0.030246
323.25	0.9628	0.037196

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors refer to the compound as 1,8-dihydroacenaphthalene, which the compiler has taken to be acenaphthene.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9763	0.02373

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[14]F. He and P. Liu, J. Chem. Eng. Data **52**, 2536 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
278.25	0.9899	0.010098
283.05	0.9878	0.012221
288.05	0.9846	0.015448
293.25	0.9810	0.018975
298.25	0.9763	0.023672
303.15	0.9710	0.028995
308.10	0.9651	0.034855
313.20	0.9573	0.042705
318.05	0.9475	0.052472
323.05	0.9361	0.063929

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors refer to the compound as 1,8-dihydroacenaphthalene, which the compiler has taken to be acenaphthene.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9812	0.01877

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9831	0.01691

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9830	0.01705

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9682	0.03176

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9756	0.02443

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9765	0.02347

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9713	0.02867

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9608	0.03922

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9710	0.02904

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9745	0.02551

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9538	0.04617

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9491	0.05089

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9560	0.04402

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
W. E. Acree, Jr., unpublished data

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9332	0.06677

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) 3,7-Dimethyl-1-octanol; $C_{10}H_{22}O$; [106-21-8]

Original Measurements:
[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9459	0.05410

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

Original Measurements:
[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9988	0.001157

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

2.8. Acenaphthene solubility data in alkoxyalcohols

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9544	0.04561

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9392	0.06082

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9400	0.05996

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9352	0.06484

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

2.9. Acenaphthene solubility data in ketones

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 2-Butanone; C_4H_8O; [78-93-3]	[9]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8693	0.1307

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

2.10. Acenaphthene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Propanenitrile; C_3H_5N; [107-12-0]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9385	0.06154

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Butanenitrile; C_4H_7N; [109-74-0]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9026	0.09737

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9641	0.03588

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) *N*-Methylformamide; C_2H_5NO; [123-39-7]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9854	0.01458

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3. Solubility of Anthracene in Organic Solvents

3.1. Critical evaluation of experimental solubility data

Volume 58 in the IUPAC Solubility Data Series[2] contained experimental solubility data for anthracene dissolved in 12 saturated hydrocarbons (hexane, heptanes, octane, hexadecane, octadecane, cyclohexane, methylcyclohexane, cyclooctane, 2,2,4-trimethylpentane, *tert*-butylcyclohexane, squalane, and decahydronaphthalene), in five aromatic hydrocarbons (benzene, methylbenzene, 1,4-dimethylbenzene, 4-isopropyl-1-methylbenzene, and 1,2,3,4-tetrahydronaphthalene), in five alkyl alkanoates (ethyl ethanoate, butyl ethanoate, dimethyl hexanedioate, diethyl hexanedioate, and dibutyl oxalate), in two dialkyl ethers (1,1-oxybisethane and 1,1-oxybisbutane) and three cyclic ethers (tetrahydrofuran, tetrahydropyrane and 1,4-dioxane), in five haloalkanes (trichloromethane, tetrachloromethane, 1-chlorobutane, 1,4-dichlorobutane, and iodoethane), one haloalkene (trichloroethene) and three haloaromatic hydrocarbons (chlorobenzene, bromobenzene, and iodobenzene), in eight alkanols (methanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 3-methyl-1-butanol, and 1-octanol), in two alkanones (propanone and 2-butanone), and in 15 miscellaneous organic solvents (ethanenitrile, carbon disulfide, acetic anhydride, dimethyl sulfoxide, nitrobenzene, aniline, pyridine, quinoline, thiophene, methoxybenzene, 1-methyl-2-pyrrolidinone, *N*,*N*-dimethylformamide, *N*,*N*-dimethylacetamide, tetramethylene sulfone, and tributyl phosphate). Except for a few select systems, the majority of the compiled solubility data was measured at either 293.15 or 298.15 K. Anthracene solubility measurements in octadecane covered the temperature range of 466–484 K, measurements in cyclohexane covered the temperature range from 298 to 402 K, measurements in tetrahydronaphthalene covered the range from 324 to 385 K, measurements in benzene covered the range from 293 K to 364 K, measurements in methylbenzene covered the range from 293 to 333 K, measurements in 1,2,3,4-tetrahydronaphthalene covered the range from 300 to 346 K, measurements in iodobenzene covered the range from 305 to 320 K, measurements in nitrobenzene covered the range from 286 to 313 K, measurements in pyridine covered the range from 293 to 359 K, and measurements in thiophene covered the range from 297 to 358 K. The compiled solubility data also included phase diagram information for binary anthracene + acenaphthene, anthracene + chrysene, anthracene + fluoranthene, and anthracene + 1,2,3,5-tetranitrobenzene mixtures. Solubility data contained in Vol. 58 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for anthracene.

After Vol. 58 appeared in print, there have been several experimental solubility studies involving anthracene dissolved in organic solvents. Acree and co-workers[16–33] have measured the solubility of anthracene in four linear alkanes (nonane through dodecane), in two dialkylbenzenes (1,2-dimethylbenzene and 1,3-dimethylbenzene), in several primary (methanol, ethanol, 1-pentanol, 2-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 1-heptanol, 2-ethyl-1-hexanol, 1-decanol, 3,7-dimethyl-1-octanol, 1,2-ethanediol, and 2,2,2-trifluoroethanol), three secondary (2-pentanol, 4-methyl-2-pentanol, and cyclopentanol) and one tertiary (2-methyl-2-propanol) alcohol(s), in four alkyl alkanoates (methyl ethanoate, propyl ethanoate, pentyl ethanoate, and methyl butanoate), in three ethers (2,2′-oxybispropane, 2-methoxy-2-methylpropane, and 1,1′-oxybis[2-methoxyethane]), in three chlorinated alkanes (dichloromethane, trichloromethane, and 1-chlorohexane) and three halogenated benzenes (chlorobenzene, fluorobenzene, and (trifluoromethyl)benzene), in five alkoxyalcohols (2-ethoxyethanol, 2-propoxyethanol, 2-isopropoxyethanol, 2-butoxyethanol, and 3-methoxy-1-butanol) and in several miscellaneous organic solvents (methyl acetoacetate, ethyl acetoacetate, ethanenitrile, propanenitrile, butanenitrile, benzonitrile, *N*,*N*-dimethylformamide, *N*,*N*-dimethylacetamide, morpholine, ethanolamine, propylene carbonate, hexanedintitrile (also called adiponitrile) and tributyl phosphate). The authors measured the solubility at only 298.15 K, and for most of the solvents there are no independent experimental measurements to compare the numerical values against.

Shayanfar *et al.*[34] measured the solubility of anthracene in binary 2,2,4-trimethylpentane + ethanol solvent mixtures at 298.2, 308.2, and 318.2 K. Since only three temperatures were studied, it is not feasible to use the three-parameter Apelblat equation to assess the internal consistency of the authors' experimental data since the equation would yield essentially a perfect fit. The observed mole fraction solubility of anthracene in ethanol reported by Shayanfar *et al.*,[34] $x_1 = 0.000505$, is approximately 9% larger than the value given by Roy *et al.*,[16] $x_1 = 0.000460$. The anthracene samples used both solubility studies were recrystallized from propanone. Shayanfar *et al.*[34] started with a sample having an initial purity of 96%. Roy *et al.*[16] started with a sample of much higher purity, 99+%.

Two research groups have determined phase diagrams for binary mixtures containing anthracene. Auolmi *et al.*[15] measured the solid-liquid equilibria data for the anthracene + hexatricontane system by a differential scanning calorimetric method. The authors employed a SSF to describe the activity coefficients of anthracene and hexatricontane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of T/K = 349.9 and eutectic mole fraction of anthracene of $x_1 = 0.038$. Lisicki and Jamróz[35] reported solid-liquid equilibria data for binary mixtures containing anthracene with *N*,*N*-dimethylacetamide, 1-methyl-2-pyrrolidone, and hexahydro-1-methyl-2*H*-azepin-2-one (also called *N*-methyl-ε-caprolactam). The anthracene + *N*,*N*-dimethylformamide and anthracene + 1-methyl-2-pyrrolidone systems both exhibited simple eutectic behavior. The published experimental liquidus curves for the latter three anthracene systems did not indicate any outlier data points.

The experimental solubility data for anthracene dissolved in the different organic solvents are given in Secs. 3.2–3.9.

3.2. Anthracene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Nonane; C_9H_{20}; [111-84-2]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9979	0.002085

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9977	0.002345

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Undecane; $C_{11}H_{24}$; [1120-21-4]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9974	0.002585

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in undecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Dodecane; $C_{12}H_{26}$; [112-40-3]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9972	0.002800

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in dodecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexatricontane; $C_{36}H_{74}$; [630-06-8]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
386.45	0.9004	0.0996
409.41	0.8114	0.1886
432.38	0.6909	0.3091
450.01	0.5922	0.4078
461.12	0.4737	0.5263
468.21	0.3986	0.6014
474.51	0.2862	0.7138
480.01	0.1978	0.8022
483.46	0.0998	0.9002
488.46	0.0000	1.0000

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of anthracene and hexatricontane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of T/K = 349.9 and eutectic mole fraction of anthracene of $x_1 = 0.038$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
Phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, purification details were not given in the paper.
(2) 98+%, Fluka Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[34]A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9988	0.001187
308.2	0.9985	0.001515
318.2	0.9982	0.001768

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 356 nm.

Source and Purity of Chemicals:
(1) 96%, Fluka Chemical Company, was recrystallized several from propanone and ethyl ethanoate before use.
(2) 99+%, Merck Chemicals, Germany, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2.7% (relative uncertainty).

3.3. Anthracene solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,2-Dimethylbenzene; C_8H_{10}; [95-47-6]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9915	0.008458

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 98+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9920	0.007956

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.4. Anthracene solubility data in esters

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9944	0.003639

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[18]L. Alcazar, A. Blanco, R. Cano, L. Fisher, M. Nau, L. Sidransky, and W. E. Acree, Jr., J. Chem. Eng. Data. **53**, 201 (2008).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9941	0.00588

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9924	0.007547

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methyl butanoate; $C_5H_{10}O_2$; [623-42-7]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9941	0.005893

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.5. Anthracene solubility data in ethers

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[19]M. Carrillo, M. Corella, K. Wolcott, K. R. Bowen, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 270 (2007).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9975	0.002515

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[20]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	$x_2{}^b$	$x_1{}^c$
1.0000	0.9969	0.003050

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9+%, Arco Chemical Company, USA, was stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[21]K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	$x_2{}^b$	$x_1{}^c$
1.0000	0.9886	0.01139

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from propanone.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, was stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.6. Anthracene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Dichloromethane; CH_2Cl_2; [75-09-2]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	$x_2{}^b$	$x_1{}^c$
1.0000	0.9061	0.009387

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9892	0.01084

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, was shaken several times with an aqueous sodium hydroxide solution and then with distilled water to remove the ethanol stabilizer. The resulting solution was dried over both anhydrous calcium chloride and molecular sieves, and then distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9928	0.007177

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9900	0.009962

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.9%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Fluorobenzene; C_6H_5F; [462-06-6]

Original Measurements:
[22]M. H. Abraham, W. E. Acree, Jr., A. J. Leo, and D. Hoekman, New J. Chem. **33**, 1685 (2009).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9932	0.006764

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

The experimental value was reported as the logarithm of anthracene's molar solubility in fluorobenzene dissolved by the solute's molar solubility in water. Experimental mole fraction solubility was obtained from the authors.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) (Trifluoromethyl)benzene; $C_7H_5F_3$; [98-08-8]

Original Measurements:
W. E. Acree, Jr., unpublished data.

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9961	0.003864

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.7. Anthracene solubility data in alcohols

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9998	0.000243

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.9+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Ethanol; C_2H_6O; [64-17-5]	**Original Measurements:** [16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9995	0.000460

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Ethanol; C_2H_6O; [64-17-5]	**Original Measurements:** [34]A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9995	0.000505
308.2	0.9993	0.000665
318.2	0.9992	0.000780

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 356 nm.

Source and Purity of Chemicals:
(1) 96%, Fluka Chemical Company, was recrystallized several from propanone and ethyl ethanoate before use.
(2) 99+%, Absolute, Merck Chemicals, Germany, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2.7% (relative uncertainty).

Components: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	**Original Measurements:** [23]K. M. De Fina, T. T. Van, A. Ibarra, E. Hamilton, J. Martinez, A. Valdez, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 249 (2001).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9996	0.000430

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[24]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9989	0.001097

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[24]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9992	0.000800

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[25]C. I. Monárrez, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1341 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9992	0.000786

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9985	0.001483

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[26]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, Jr., V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9990	0.000996

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was recrystallized several times from propanone before use.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[24]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9992	0.000779

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Heptanol; $C_7H_{16}O$; [111-27-3]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9981	0.001869

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[27]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, P. Otero, M. Jayasekera, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1270 (1995).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9986	0.001397

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[28]W. E. Acree, Jr. and M. H. Abraham, Can. J. Chem. **79**, 1466 (2001).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9966	0.003433

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

The experimental value was reported as the molar solubility of anthracene in 1-decanol. Mole fraction solubility was provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3,7-Dimethyl-1-octanol; $C_{10}H_{22}O$; [106-21-8]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9980	0.002001

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9987	0.001330

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9999	0.0000715

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]	[16] L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9999	0.0000865

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.8. Anthracene solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[29] C. E. Hernández, L. E. Roy, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 677 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9971	0.002921

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[30] C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Jackson, G. Brown, and W. E. Acree, Jr., Chem. Eng. Commun. **169**, 137 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9967	0.003343

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[31]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Jackson, G. Brown, T. L. Borders, J. T. Sanders, and W. E. Acree, Jr., Phys. Chem. Liq. **36**, 257 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9969	0.003093

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[32]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9962	0.003785

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[33]C. E. Hernández, L. E. Roy, G. D. Reddy, T. L. Borders, J. T. Sanders, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 31 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9973	0.002702

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.9. Anthracene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methyl acetoacetate; $C_5H_8O_3$; [105-45-3]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9968	0.003191

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:.**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Ethyl acetoacetate; $C_6H_{10}O_3$; [141-97-9]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999)
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9955	0.004533

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9992	0.000830

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Propanenitrile; C_3H_5N; [107-12-0]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9971	0.002879

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Butanenitrile; C_4H_7N; [109-74-0]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9955	0.004527

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Benzonitrile; C_7H_5N; [100-47-0]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9916	0.008426

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [111-84-2]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9922	0.007839

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[16]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9873	0.01267

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
299.5	0.9900	0.0100
318.3	0.9802	0.0198
332.2	0.9699	0.0301
350.3	0.9498	0.0502
363.1	0.9301	0.0699
378.9	0.8979	0.1021
398.6	0.8504	0.1496
408.7	0.8144	0.1856
418.0	0.7760	0.2240
422.9	0.7506	0.2494
431.5	0.6991	0.3009
446.0	0.5989	0.4011

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 250.3$ as determined by calorimetric measurements. The eutectic composition was not determined.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 99.9%, Heybreck, Switzerland, was used as received.
(2) Purest grade, Merck-Schuchardt, Federal Republic of Germany, was distilled under reduced pressure and dried over molecular sieves to produce a sample of 99.9% purity (mass percent).

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
272.9	0.9892	0.0108
296.3	0.9799	0.0201
318.1	0.9700	0.0300
333.4	0.9497	0.0503
344.7	0.9395	0.0605
361.2	0.9090	0.0910
381.3	0.8698	0.1302
393.7	0.8299	0.1701
403.7	0.7994	0.2006
418.0	0.9497	0.2503
438.7	0.6698	0.3302
451.1	0.5888	0.4112
461.4	0.4995	0.5005
471.0	0.3998	0.6002
477.5	0.2990	0.7010

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 245.1$ as determined by calorimetric measurements. The eutectic composition was not determined.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 99.9%, Heybreck, Switzerland, was used as received.
(2) Technical Grade, BASF, Federal Republic of Germany, was purified by treatment with a 2% solution of potassium permanganate, and then distilled under reduced pressure to collect the distillate having 99.8% purity (mass percent). The purified sample was dried over molecular sieves.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexahydro-1-methyl-2*H*-azepin-2-one (*N*-Methyl-ε-caprolactam); $C_7H_{13}NO$; [2556-73-2]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
279.6	1.0000	0.0000
287.4	0.9905	0.0095
309.0	0.9696	0.0304
322.9	0.9601	0.0399
332.4	0.9491	0.0509
349.1	0.9281	0.0719
356.1	0.9195	0.0805
364.3	0.9016	0.0984
377.8	0.8777	0.1223
389.4	0.8469	0.1531
405.5	0.7948	0.2052
424.9	0.7004	0.2996
439.9	0.5993	0.4007
453.2	0.4999	0.5001
460.2	0.3990	0.6010
466.6	0.3003	0.6997
472.9	0.2012	0.7988
480.1	0.0994	0.9006
489.4	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 99.9%, Heybreck, Switzerland, was used as received.
(2) Technical Grade, Leuna Werke, Federal Republic of Germany, was purified by super-rectification and then dried over molecular sieves to give a sample having a purity of 99.9% by mass.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]	W. E. Acree, Jr.,
(2) Morpholine; C_4H_9NO; [110-91-8]	unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9918	0.008193

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution
[b] x_1: mole fraction solubility of the solute
[c] x_2: mole fraction of component 2 in the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]	W. E. Acree, Jr.,
(2) Ethanolamine; C_2H_7NO; [141-43-5]	unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9997	0.0002587

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]	W. E. Acree, Jr.,
(2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9979	0.002102

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]	W. E. Acree, Jr.,
(2) Hexanedinitrile; $C_6H_8N_2$; [111-69-3]	unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9972	0.002801

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]	W. E. Acree, Jr.,
(2) Tributyl phosphate; $C_{12}H_{27}O_4P$; [126-73-8]	unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9850	0.01498

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from propanone.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

4. Solubility of Biphenyl in Organic Solvents

4.1. Critical evaluation of experimental solubility data

Volume 58 in the IUPAC Solubility Data Series[2] contained experimental solubility data for biphenyl in three linear alkanes (hexane, heptane and octane) and eight cycloalkanes (cyclohexane, methylcyclohexane, *cis*-1,2-dimethylcyclohexane, *trans*-1,2-dimethylcyclohexane, *cis*-1,3-dimethylcyclohexane, *cis*-1,4-dimethylcyclohexane, *trans*-1,2-dimethylcyclohexane, and decahydronaphthalene), in four aromatic hydrocarbons (benzene, methylbenzene, ethylbenzene and 1,2,3,4-tetrahydronaphthalene), in one cyclic ether (1,4-dioxane), in six halogenated alkanes (dichloromethane, trichloromethane, tetrachloromethane, 1,2-dibromethane, 1,1-dichloroethane, and 1,2-dichloroethane) and two halogenated benzenes (chlorobenzene and hexachlorobenzene), in one alkanol (1-octanol) and four miscellaneous organic solvents (carbon disulfide, pyridine, thiophene and nitrobenzene). For several of the solvents, the reporting authors made measurements at more than one temperature. Biphenyl solubility data in both hexane and octane covered the temperature range from 298 to 313 K, data in heptane, cyclohexane, benzene, carbon tetrachloride, carbon disulfide, pyridine, and thiophene covered the range from about 298 to 335 K, data in decahydronaphthalene and 1,2,3,4-tetrahydronaphthalene covered the range from about 309 to 328 K, data in 1,4-dioxane covered the range from 300 to 341 K, and data for hexafluorobenzene covered the range from 307 to 337 K. The compiled solubility data also included phase diagram information for binary biphenyl + tetracosane, biphenyl + octacosane, biphenyl + naphthalene, biphenyl + 2-methylnaphthalene, biphenyl + 2,6-dimethylnaphtalene, biphenyl + 1,2-diphenylethane, diphenyl + diphenyl ether, biphenyl + 1-octadecanol, biphenyl + indole, biphenyl + diphenylamine, and biphenyl + octadecanoic acid mixtures. Solubility data contained in Vol. 58 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for biphenyl.

A search of the published chemical and engineering literature covering the period of 1995 to 2011 found only two solubility studies involving biphenyl and one study reporting the phase diagrams for two binary systems containing biphenyl. De Fina *et al.*[36] determined the solubility of biphenyl at 298.15 K in 26 different alkane, dialkyl ether and alcohol solvents based on a spectrophotometric method. Grubbs *et al.*[37] later measured the solubility of biphenyl in five alkoxyalcohols (2-ethoxyethanol, 2-propoxyethanol, 2-isopropoxyethanol, 2-butoxyethanol, and 3-methoxy-1-butanol) at 298.15 K. It is not possible to conduct a critical evaluation of these two sets of published biphenyl solubility data because independent values are not available, and because the measurements were performed at only a single temperature. Phase diagrams of the binary biphenyl + octadecane and biphenyl + naphthalene systems were reported by Mengarelli *et al.*[38] Freezing-point temperatures for the biphenyl + naphthalene system were in good agreement with calculated values assuming an ideal solution. In the case of the binary biphenyl + octadecane system, the authors noted that activity coefficients of the polycyclic aromatic hydrocarbon solute, calculated from the freezing point temperatures, differed by 2% from calculated values using Flory's model with regular solution residual contribution and a 2/3 exponent in the definition of the volume fraction.

The experimental solubility data for biphenyl dissolved in the different organic solvents are given in Secs. 4.2–4.7.

4.2. Biphenyl solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Nonane; C_9H_{20}; [111-84-2]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8449	0.1551

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$	x_2	x_1
1.0000	0.8364	0.1636

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).

Variables:
$T/\mathrm{K} = 298.15$

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.7849	0.2151

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Octadecane; $C_{18}H_{38}$; [593-45-3]

Original Measurements:
[38]A. C. Mengarelli, S. B. Bottini, and E. A. Brignole, J. Chem. Eng. Data **40**, 746 (1995).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
301.25	1.000	0.000
299.60	0.845	0.155
299.12	0.775	0.225
298.81	0.754	0.246
298.77	0.748	0.252
298.57	0.734	0.266
303.86	0.708	0.292
312.25	0.645	0.355
317.60	0.586	0.414
324.95	0.476	0.524
328.75	0.378	0.622
332.22	0.288	0.712
334.21	0.206	0.794
336.57	0.132	0.868
338.77	0.063	0.937
341.62	0.000	1.000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Thermostatted liquid bath, platinum resistance thermometer, and a coiled wire driven by a small electrical motor to provide stirring.
A liquid mixture of known composition was prepared by mass and placed in a glass tube. The solution was slowly cooled until a solid phase appeared. The temperature of the solution was recorded continuously with a platinum resistance thermometer. A break point in the temperature versus time curve indicated formation of a solid phase. The temperature at break point was taken to be the solid-liquid equilibrium temperature, and the composition of the solution gives the solubility of the crystalline solute in the liquid solvent.

Source and Purity of Chemicals:
(1) Chemical purity and source not given in the paper.
(2) 97%, Aldrich Chemical Company, Milwaukee, WI, USA, purification details were not given in the paper.

Estimated Error:
Temperature: ±0.5 K.
x_1: ± 0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.7806	0.2194

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

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

Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.

(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.8906	0.1094

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

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

Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.

(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.8260	0.1740

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

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

Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.

(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

4.3. Biphenyl solubility data in aromatic hydrocarbons

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Naphthalene; $C_{10}H_8$; [91-20-3]

Original Measurements:
[38]A. C. Mengarelli, S. B. Bottini, and E. A. Brignole, J. Chem. Eng. Data **40**, 746 (1995).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
351.88	1.00	0.00
347.49	0.92	0.08
342.42	0.83	0.17
336.26	0.74	0.26
329.50	0.64	0.36
321.50	0.55	0.45
317.69	0.50	0.50
312.20	0.44	0.56
316.15	0.39	0.61
320.99	0.34	0.66
328.76	0.23	0.77
335.20	0.12	0.88
341.62	0.00	1.00

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Thermostatted liquid bath, platinum resistance thermometer, and a coiled wire driven by a small electrical motor to provide stirring.
A liquid mixture of known composition was prepared by mass and placed in a glass tube. The solution was slowly cooled until a solid phase appeared. The temperature of the solution was recorded continuously with a platinum resistance thermometer. A break point in the temperature versus time curve indicated formation of a solid phase. The temperature at break point was taken to be the solid-liquid equilibrium temperature, and the composition of the solution gives the solubility of the crystalline solute in the liquid solvent.

Source and Purity of Chemicals:
(1) Chemical purity and source not given in the paper.
(2) Chemical purity and source not given in the paper.

Estimated Error:
Temperature: ±0.5 K.
x_1: ± 0.01 (estimated by compiler).

4.4. Biphenyl solubility data in ethers

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

Original Measurements:
[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.7340	0.2660

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]

Original Measurements:
W. E. Acree, Jr., unpublished data.

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.7150	0.2850

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

4.5. Biphenyl solubility data in alcohols

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Methanol; CH_4O; [67-56-1]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9815	0.01851

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Ethanol; C_2H_6O; [64-17-5]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9654	0.03456

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Propanol; C_3H_8O; [71-23-8]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9538	0.04620

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Propanol; C_3H_8O; [67-63-0]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9647	0.03533

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9421	0.05788

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9499	0.05005

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9609	0.03906

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9588	0.04118

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Arco Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9243	0.07573

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9347	0.06525

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9434	0.05664

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9288	0.07120

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9141	0.08592

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9278	0.07216

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9388	0.06115

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.8999	0.1001

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.8903	0.1097

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9052	0.09481

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[36]K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9973	0.00269

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

4.6. Biphenyl solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [111-27-3]	[37]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8589	0.1411

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol or 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[37]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8317	0.1683

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol or 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[37]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8387	0.1613

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol or 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[37]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8449	0.1551

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol or 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[37]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8536	0.1464

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol or 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

4.7. Biphenyl solubility data in miscellaneous organic solvents

Components:	Original Measurements:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8700	0.1300

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 250 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

5. Solubility of Carbazole in Organic Solvents

5.1. Critical evaluation of experimental solubility data

Volume 58 in the IUPAC Solubility Data Series[2] contained experimental solubility data for carbazole dissolved in 13 saturated hydrocarbons (hexane, heptane, octane, decane, dodecane, hexadecane, cyclohexane, methylcyclohexane, cyclooctane, 2,2,4-trimethylpentane, *tert*-butylcyclohexane, squalane, and decahydronapthalene), in three aromatic hydrocarbons (benzene, methylcyclohexane, and 1,4-dimethylbenzene), in two alkyl alkanoates (ethyl ethanoate and butyl butanoate), in seven ethers (1,1′-oxybisethane, 1,1′-oxybisbutane, 1,1′-oxybispentane, tetrahydropyran, tetrahydrofuran, 1,4-dioxane, and methoxybenzene), in six chloroalkanes (trichloromethane, tetrachloromethane, 1-chlorohexane, 1-chlorooctane, 1-chlorotetradecane, and chlorocyclohexane), in seven alkanols (methanol, ethanol, 1-propanol, 2-propnaol, 1-butanol, 1-octanol, and 1,2-ethanediol), in three alkanones (propanone, butanone, and cyclohexanone) and in acetophenone, and in 11 miscellaneous organic solvents (carbon disulfide, pyridine, quinoline, thiophene, dimethyl sulfoxide, nitromethane, acetic anhydride, 1-methyl-2-pyrrolidinone, *N*,*N*-dimethylacetamide, *N*,*N*-dimethylformamide, tetramethylene sulfone, and tributyl phosphate). Except for cyclohexane, decahydronaphthalene, benzene, methylbenzene 1,2,3,4-tetrahydronaphthalene, tetrachloromethane, 2-propanol, pyridine, and thiophene, solubility measurements were made at only a single temperature of 298 K, or at a single ambient temperature estimated at between 298 and 303 K. Solubility measurements in methylbenzene, tetrachloromethane, and 2-propanol covered 40 K in temperature from 293 to 333 K. Solubility data for carbazole in cyclohexane (from 293 to 357 K), decahydronaphthalene (from 333 to 502 K), 1,2,3,4-tetrahydronaphthalene (from 345 to 495 K), and pyridine (from 302 to 439 K) covered a much larger temperature interval, albeit measurements were made at only a few temperatures within the given interval. Solubility data contained in Vol. 58 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for carbazole.

There has been very little carbazole solubility data published during the last 17 years. The only data that could be found pertained to phase diagrams determined by Lisicki and Jamróz[35] for carbazole + *N*,*N*-dimethylacetamide, carbazole + 1-methyl-2-pyrrolidone, and carbazole + hexahydro-1-methyl-2*H*-azepin-2-one (also called *N*-methyl-ε-caprolactam). The published experimental liquidus curves for the latter three carbazole systems did not indicate any outlier data points. The experimental data are listed in Sec. 5.2.

5.2. Carbazole solubility data in miscellaneous organic solvents

Components: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	**Original Measurements:** [35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
253.2	1.0000	0.0000
253.0	0.9898	0.0102
252.1	0.9779	0.0221
251.6	0.9690	0.0310
251.3	0.9597	0.0403
256.2	0.9472	0.0528
269.1	0.9252	0.0748
285.3	0.8825	0.1175
291.7	0.8584	0.1416
302.8	0.8217	0.1783
311.3	0.7801	0.2199
311.4	0.7786	0.2214
317.5	0.7491	0.2509
318.7	0.7416	0.2584
321.2	0.7284	0.2716
331.5	0.7185	0.2815
343.8	0.7033	0.2967
359.3	0.6790	0.3210
363.3	0.6737	0.3263
377.4	0.6490	0.3510
398.1	0.6101	0.3899
411.9	0.5773	0.4227
420.9	0.5567	0.4433
444.3	0.4842	0.5158
518.7	0.0000	1.0000

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the data reveal the presence of a eutectic point at a carbazole mole fraction of $x_1 = 0.0475$ and eutectic temperature of $T/\mathrm{K} = 250.8$. An incongruent melting temperature of $T/\mathrm{K} = 322.8$ and $x_1 = 0.27$ suggested formation of a 1:1 carbazole–*N*,*N*-dimethylacetamide molecular complex.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was purified by melting with potassium hydroxide, followed by repeated recrystallization from dimethylbenzene to yield a sample having a purity of 99.9% (by mass).
(2) Purest grade, Merck-Schuchardt, was distilled under reduced pressure and dried over molecular sieves to produce a sample of 99.9% purity (mass percent).

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	**Original Measurements:** [35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
248.5	1.0000	0.0000
252.7	0.9941	0.0059
260.2	0.9902	0.0098
268.7	0.9804	0.0196
284.1	0.9520	0.0480
296.4	0.9090	0.0910
299.6	0.8935	0.1065
302.2	0.8750	0.1250
306.9	0.8371	0.1629
309.8	0.8097	0.1903
312.7	0.8000	0.2000
319.2	0.7778	0.2222
324.5	0.7499	0.2501
330.5	0.7140	0.2860
334.2	0.6875	0.3125
353.7	0.6667	0.3333
373.4	0.6360	0.3640
393.3	0.6002	0.3998
418.1	0.5499	0.4501
437.2	0.5003	0.4997
456.3	0.4398	0.5602
518.7	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the binary system has two incongruent melting temperatures: the first at T/K $= 309.2$ and a carbazole mole fraction of $x_1 = 0.189$, and the second at T/K $= 334.5$ and $x_1 = 0.313$. The composition of the complexes could not be established explicitly. An eutectic temperature of T/K $=$ 241.3 was determined based on calorimetric measurements.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was purified by melting with potassium hydroxide, followed by repeated recrystallization from dimethylbenzene to yield a sample having a purity of 99.9% (by mass).
(2) Technical Grade, BASF, Federal Republic of Germany, was purified by treatment with a 2% solution of potassium permanganate, and then distilled under reduced pressure to collect the distillate having 99.8% purity (mass percent). The purified sample was dried over molecular sieves.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Hexahydro-1-methyl-2*H*-azepin-2-one (*N*-Methyl-ε-caprolactam); $C_7H_{13}NO$; [2556-73-2]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
279.6	1.0000	0.0000
282.7	0.7489	0.2511
306.4	0.7284	0.2716
322.1	0.7111	0.2889
332.0	0.6930	0.3070
341.9	0.6793	0.3207
363.0	0.6459	0.3541
394.3	0.5998	0.4002
398.4	0.5910	0.4090
422.1	0.5417	0.4583
439.3	0.4909	0.5091
462.4	0.4012	0.5988
463.2	0.3975	0.6025
481.7	0.3009	0.6991
496.8	0.1996	0.8004
508.8	0.0988	0.9012
518.7	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was purified by melting with potassium hydroxide, followed by repeated recrystallization from dimethylbenzene to yield a sample having a purity of 99.9% (by mass).
(2) Technical Grade, Leuna Werke, Federal Republic of Germany, was purified by super-rectification and then dried over molecular sieves to give a sample having a purity of 99.9% by mass.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

TABLE 2. Parameters of the Apelblat equation for describing the solubility of dibenzofuran in various organic solvents

Solvent	*A*	*B*	*C*	MRD (%)
Methylbenzene	40.193	−4126.3	−4.863	1.3
Ethyl ethanoate	36.051	−4126.4	−4.151	1.9
2,2′-Oxybispropane	20.096	−4126.8	−1.421	1.8
Tetrachloromethane	33.557	−4126.5	−3.725	1.7
Ethanol	−13.514	−4127.5	4.258	10.9
1-Butanol	−14.149	−4127.5	4.410	10.1

6. Solubility of Dibenzofuran in Organic Solvents

6.1. Critical evaluation of experimental solubility data

The dibenzofuran solubility data that was contained in Vol. 58 of the IUPAC Solubility Data Series[2] was very limited. The solubility data included mole fraction solubilities of dibenzofuran in cyclohexane (from 328 to 345 K), decahydronaphthalene (from 326 to 337 K), benzene (from 322 to 339 K), 1,2,3,4-tetrahydronaphthalene (from 319 to 340 K), pyridine (from 324 to 341 K), and thiophene (from 314 to 341 K) measured by Coon *et al.*,[39] along with the published solid-liquid equilibrium data for the binary dibenzofuran + benzene phase diagram from a paper by Domanska *et al.*[40] Solubility data contained in Vol. 58 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for dibenzofuran.

There have been three studies that have reported solubility data for dibenzofuran in organic solvents after Vol. 58 was published in 1995. First, Wei *et al.*[41] determined the solubility of dibenzofuran in methylbenzene, ethyl ethanoate, tetrachloromethane, 2,2′-oxybispropane, ethanol, and 1-butanol from 283.15 to 333.15 K. The internal consistency of the six datasets of measured dibenzofuran solubilities were assessed by curve-fitting the measured the mole fraction solubility to Eq. (3). The numerical values of the equation coefficients (*A*, *B*, and *C*) are given in Table 2, along with the respective MRDs. Examination of the numerical entries in the last column of Table 2 reveals that the largest mean relative percent deviation between the back-calculated values based on Eq. (3) and experimental data is less than 2% for the four nonalkanol solvents, which is less than the experimental uncertainties in the measured values. Much larger mean relative percent deviations of 10.9% and 10.1% were noted for ethanol and 1-butanol, respectively. The experimental uncertainties associated with solubility data for the two alcohol solvents were on the order of ±6%. Results of the mathematical representation analyses indicate that the experimental data for the first four dibenzofuran-organic solvent systems are internally consistent. Deviations for ethanol and 1-butanol are larger than desired; however, given the experimental uncertainty in the measured values they are still considered to fall within an "acceptable" level.

The final two studies involved determination of phase diagrams. Hafsaoui and Mahmound[42] used a differential scanning calorimetric method in determining solid-liquid equilibrium data for the dibenzofuran + pentacosane system. Lisicki and Jamróz[35] reported solid-liquid equilibria data for binary mixtures containing dibenzofuran with *N*,*N*-dimethylacetamide, 1-methyl-2-pyrrolidone, and hexahydro-1-methyl-2*H*-azepin-2-one (also called *N*-methyl-ε-caprolactam). The dibenzofuran + *N*,*N*-dimethylformamide and dibenzofuran + 1-methyl-2-pyrrolidone systems both exhibited simple eutectic behavior. The published experimental liquidus curves for the latter three dibenzofuran systems did not indicate any outlier data points.

The experimental solubility data for dibenzofuran dissolved in the different organic solvents are given in Secs. 6.2–6.8.

6.2. Dibenzofuran solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) Pentacosane; $C_{25}H_{52}$; [629-99-2]	[42]S. L. Hafsaoui and R. Mahmoud, J. Therm. Anal. Calorim. **88**, 565 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
324.10	1.000	0.000
323.65	0.901	0.099
322.35	0.798	0.202
319.34	0.702	0.298
326.43	0.601	0.399
332.21	0.501	0.499
337.75	0.399	0.601
344.04	0.299	0.701
348.94	0.199	0.801
352.84	0.101	0.899
355.10	0.000	1.000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
Mixtures of dibenzofuran and pentacosane were prepared by mass. The resulting mixtures were heated slowly with agitation until the entire sample melted. After melting the sample was immersed in liquid nitrogen to solidify the mixture completely. A small amount of solid was removed and sealed in a pan, the capsule was crimped, and placed in the calorimetric block of the differential scanning calorimeter for analysis.

Source and Purity of Chemicals:
(1) 98%, Fluka Chemical Company, was used as received.
(2) 99%, Fluka Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.7 K.
x_1: ±0.002 (estimated by compiler).

6.3. Dibenzofuran solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) Methylbenzene; C_7H_8; [108-88-3]	[41]Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.8423	0.1577
288.15	0.8145	0.1855
293.15	0.7769	0.2231
298.15	0.7344	0.2656
303.15	0.6987	0.3013
308.15	0.6563	0.3437
313.15	0.6009	0.3991
318.15	0.5453	0.4547
323.15	0.4855	0.5145
328.15	0.4183	0.5817
333.15	0.3762	0.6238

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed vessel, thermostatted bath and gas chromatograph equipped with a flame ionization detector.
The authors' description states that the method is based on adding excess solute to a stirred solution kept at fixed temperature for at least 24 h. After stirring was stopped, the solid was allowed to settle to the bottom of the container. Three samples of about 10 mL each were carefully withdrawn and filtered through a 0.045 μm PTFE filter. The filtered samples were then analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Chemicals:
(1) 99.5% (by gas chromatography), Tianjin Kewei Chemical Reagents, Company, Ltd., China, recrystallized twice. Recrystallization solvent was not specified.
(2) 99.5%, Analytical Reagent Grade, Tianjin Damao Chemical Reagent Company, China, was used without further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

6.4. Dibenzofuran solubility data in esters

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[41]Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.8545	0.1455
288.15	0.8321	0.1679
293.15	0.8011	0.1989
298.15	0.7685	0.2315
303.15	0.7315	0.2685
308.15	0.6723	0.3277
313.15	0.6128	0.3872
318.15	0.5589	0.4411
323.15	0.4983	0.5017
328.15	0.4349	0.5651
333.15	0.3751	0.6249

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed vessel, thermostatted bath and gas chromatograph equipped with a flame ionization detector.
The authors' description states that the method is based on adding excess solute to a stirred solution kept at fixed temperature for at least 24 h. After stirring was stopped, the solid was allowed to settle to the bottom of the container. Three samples of about 10 mL each were carefully withdrawn and filtered through a 0.045 μm PTFE filter. The filtered samples were then analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Chemicals:
(1) 99.5% (by gas chromatography), Tianjin Kewei Chemical Reagents, Company, Ltd., China, recrystallized twice. Recrystallization solvent was not specified.
(2) 99.5%, Analytical Reagent Grade, Tianjin Damao Chemical Reagent Company, China, was used without further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

6.5. Dibenzofuran solubility data in ethers

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[41]Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.9162	0.0838
288.15	0.8958	0.1042
293.15	0.8698	0.1302
298.15	0.8452	0.1548
303.15	0.8168	0.1832
308.15	0.7634	0.2366
313.15	0.7155	0.2845
318.15	0.6589	0.3411
323.15	0.5881	0.4119
328.15	0.4919	0.5081
333.15	0.4202	0.5798

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed vessel, thermostatted bath and gas chromatograph equipped with a flame ionization detector.
The authors' description states that the method is based on adding excess solute to a stirred solution kept at fixed temperature for at least 24 h. After stirring was stopped, the solid was allowed to settle to the bottom of the container. Three samples of about 10 mL each were carefully withdrawn and filtered through a 0.045 μm PTFE filter. The filtered samples were then analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Chemicals:
(1) 99.5% (by gas chromatography), Tianjin Kewei Chemical Reagents, Company, Ltd., China, recrystallized twice. Recrystallization solvent was not specified.
(2) 99.5%, Analytical Reagent Grade, Tianjin Damao Chemical Reagent Company, China, was used without further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

6.6. Dibenzofuran solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) Tetrachloromethane; CCl_4; [56-23-5]	[41]Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.8661	0.1339
288.15	0.8386	0.1614
293.15	0.8087	0.1913
298.15	0.7842	0.2158
303.15	0.7361	0.2639
308.15	0.6934	0.3066
313.15	0.6458	0.3542
318.15	0.5881	0.4119
323.15	0.5086	0.4914
328.15	0.4521	0.5479
333.15	0.3652	0.6348

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed vessel, thermostatted bath and gas chromatograph equipped with a flame ionization detector.
The authors' description states that the method is based on adding excess solute to a stirred solution kept at fixed temperature for at least 24 h. After stirring was stopped, the solid was allowed to settle to the bottom of the container. Three samples of about 10 mL each were carefully withdrawn and filtered through a 0.045 μm PTFE filter. The filtered samples were then analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Chemicals:
(1) 99.5% (by gas chromatography), Tianjin Kewei Chemical Reagents, Company, Ltd., China, recrystallized twice. Recrystallization solvent was not specified.
(2) 99.5%, Analytical Reagent Grade, Tianjin Damao Chemical Reagent Company, China, was used without further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

6.7. Dibenzofuran solubility data in alcohols

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) Ethanol; C_2H_6O; [64-17-5]	[41]Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.9789	0.0211
288.15	0.9729	0.0271
293.15	0.9678	0.0322
298.15	0.9586	0.0414
303.15	0.9511	0.0489
308.15	0.9293	0.0707
313.15	0.8977	0.1023
318.15	0.8659	0.1341
323.15	0.8029	0.1971
328.15	0.7169	0.2831
333.15	0.6659	0.3341

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed vessel, thermostatted bath and gas chromatograph equipped with a flame ionization detector.
The authors' description states that the method is based on adding excess solute to a stirred solution kept at fixed temperature for at least 24 h. After stirring was stopped, the solid was allowed to settle to the bottom of the container. Three samples of about 10 mL each were carefully withdrawn and filtered through a 0.045 μm PTFE filter. The filtered samples were then analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Chemicals:
(1) 99.5% (by gas chromatography), Tianjin Kewei Chemical Reagents, Company, Ltd., China, recrystallized twice. Recrystallization solvent was not specified.
(2) 99.5%, Analytical Reagent Grade, Tianjin Damao Chemical Reagent Company, China, was used without further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±6% (relative error).

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[41] Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.9719	0.0281
288.15	0.9674	0.0326
293.15	0.9579	0.0421
298.15	0.9469	0.0531
303.15	0.9329	0.0671
308.15	0.9123	0.0877
313.15	0.8932	0.1068
318.15	0.8336	0.1664
323.15	0.7699	0.2301
328.15	0.6362	0.3638
333.15	0.4859	0.5141

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed vessel, thermostatted bath and gas chromatograph equipped with a flame ionization detector
The authors' description states that the method is based on adding excess solute to a stirred solution kept at fixed temperature for at least 24 h. After stirring was stopped, the solid was allowed to settle to the bottom of the container. Three samples of about 10 mL each were carefully withdrawn and filtered through a 0.045 μm PTFE filter. The filtered samples were then analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Chemicals:
(1) 99.5% (by gas chromatography), Tianjin Kewei Chemical Reagents, Company, Ltd., China, recrystallized twice. Recrystallization solvent was not specified.
(2) 99.5%, Analytical Reagent Grade, Tianjin Damao Chemical Reagent Company, China, was used without further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±6% (relative error).

6.8. Dibenzofuran solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[35] Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
253.2	1.0000	0.0000
252.8	0.9894	0.0106
252.4	0.9779	0.0221
251.7	0.9654	0.0346
249.5	0.9462	0.0538
247.9	0.9305	0.0695
249.6	0.9137	0.0863
256.7	0.8915	0.1085
272.7	0.8227	0.1773
283.4	0.7723	0.2277
298.9	0.6764	0.3236
313.4	0.5765	0.4235
323.2	0.4745	0.5255
332.7	0.3584	0.6416
337.7	0.3003	0.6997
344.3	0.2084	0.7916
351.0	0.1021	0.8979
354.1	0.0546	0.9454
355.8	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 247.3$ and eutectic composition of $x_1 = 0.079$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Purest grade, Merck-Schuchardt, was distilled under reduced pressure and dried over molecular sieves to produce a sample of 99.9% purity (mass percent).

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
248.5	1.0000	0.0000
247.9	0.9709	0.0291
247.6	0.9648	0.0352
244.8	0.9047	0.0953
244.3	0.8791	0.1209
243.0	0.8580	0.1420
247.3	0.8434	0.1566
249.0	0.8399	0.1601
252.7	0.8275	0.1725
258.3	0.8115	0.1885
270.1	0.7716	0.2284
286.3	0.7009	0.2991
301.4	0.6200	0.3800
317.1	0.5125	0.4875
327.3	0.4094	0.5906
335.8	0.3210	0.6790
342.9	0.2336	0.7664
352.1	0.1074	0.8926
353.4	0.0675	0.9325
355.8	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 242.1$ and eutectic composition of $x_1 = 0.141$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Technical Grade, BASF, Federal Republic of Germany, was purified by treatment with a 2% solution of potassium permanganate, and then distilled under reduced pressure to collect the distillate having 99.8% purity (mass percent). The purified sample was dried over molecular sieves.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9] (2) Hexahydro-1-methyl-2*H*-azepin-2-one (*N*-Methyl-ε-caprolactam); $C_7H_{13}NO$; [2556-73-2]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
279.6	1.0000	0.0000
286.3	0.7030	0.2970
296.6	0.6479	0.3521
305.7	0.6049	0.3951
306.3	0.5977	0.4023
314.1	0.5495	0.4505
320.2	0.5056	0.4944
329.9	0.4110	0.5890
330.9	0.3998	0.6002
337.9	0.3141	0.6859
345.5	0.2093	0.7907
351.8	0.0888	0.9112
355.8	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Temperature controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Technical Grade, Leuna Werke, Federal Republic of Germany, was purified by super-rectification and then dried over molecular sieves to give a sample having a purity of 99.9% by mass.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

7. Solubility of Dibenzothiophene in Organic Solvents

7.1. Critical evaluation of experimental solubility data

The dibenzothiophene solubility data that was contained in Vol. 58 of the IUPAC Solubility Data Series[2] was very limited. The solubility data included mole fraction solubilities of dibenzothiophene in cyclohexane (from 321 to 343 K), decahydronaphthalene (from 311 to 334 K), benzene (from 310 to 342 K), 1,2,3,4-tetrahydronaphthalene (from 309 to 338 K), pyridine (from 307 to 335 K), and thiophene (from 309 to 337 K) measured by Coon *et al.*,[39] along with the published solid-liquid equilibrium data for the binary dibenzothiophene + benzene phase diagram from a paper by Domanska *et al.*[40] Solubility data contained in Vol. 58 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for dibenzothiophene.

A search of the published chemical and engineering literature from 1995 to 2011 found two papers reporting experimental dibenzothiophene solubility data. Ramirez-Verduzco *et al.*[43] determined the solubility of dibenzothiophene in cyclohexane, tetradecane, hexadecane, dihydro-2(3*H*)-furanone (commonly referred to as γ-butyrolactone), and acetonitrile as a function of temperature. Each of the five systems covered a temperature range of more than 40 K. The authors noted that their experimental results for the dibenzothiophene + cyclohexane system were in good agreement with corresponding values previously reported by Coon *et al.*[39] The highest deviation noted in the solid-liquidus temperature was 1.2 K. The experimental data were correlated with both the two-parameter Wilson and UNIQUAC models. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. Absolute average relative deviations between calculated and observed values were less than 3%.

Lisicki and Jamróz[35] reported solid-liquid equilibria data for binary mixtures containing dibenzothiophene with *N*,*N*-dimethylacetamide, 1-methyl-2-pyrrolidone and hexahydro-1-methyl-2*H*-azepin-2-one (also called *N*-methyl-ε-caprolactam). The dibenzothiophene + *N*,*N*-dimethylformamide and dibenzothiophene + 1-methyl-2-pyrrolidone systems both exhibited simple eutectic behavior. The published experimental liquidus curves for the latter three dibenzothiophene systems did not indicate any outlier data points.

The experimental solubility data for dibenzothiophene dissolved in the different organic solvents are given in Secs. 7.2–7.4.

7.2. Dibenzothiophene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Tetradecane; $C_{14}H_{30}$; [629-59-4]	[43]L. F. Ramirez-Verduzco, A. Rojas-Aguilar, J. A. De los Reyes, J. A. Munoz-Arroyo, and F. Murrieta-Guevara, J. Chem. Eng. Data **52**, 2212 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.2	0.9770	0.0230
283.9	0.9700	0.0300
291.0	0.9600	0.0400
298.3	0.9475	0.0525
316.1	0.9041	0.0959
337.2	0.7965	0.2035
346.7	0.7018	0.2982
352.6	0.5993	0.4007
356.2	0.5035	0.4965

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the eutectic point occurred at $x_1 = 0.0230$ and T/K $= 278.2$.

Auxiliary Information

Method/Apparatus/Procedure:
Heating circulating bath and platinum resistance temperature probe. Synthetic mixtures of known compositions were prepared by mass. Samples were slowly heated in a temperature bath, and the temperature at which the last amount of solid solute dissolved was measured. The temperature obtained was taken to represent the saturation point for the mixture being studied.

Source and Purity of Chemicals:
(1) 98.0%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.0%, Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[43]L. F. Ramirez-Verduzco, A. Rojas-Aguilar, J. A. De los Reyes, J. A. Munoz-Arroyo, and F. Murrieta-Guevara, J. Chem. Eng. Data **52**, 2212 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
291.1	0.9939	0.0061
290.9	0.9816	0.0184
290.8	0.9695	0.0305
290.6	0.9573	0.0427
290.6	0.9561	0.0439
290.7	0.9549	0.0451
291.0	0.9537	0.0463
292.2	0.9525	0.0475
293.0	0.9503	0.0497
293.7	0.9496	0.0504
304.4	0.9274	0.0726
315.0	0.8992	0.1008
319.9	0.8799	0.1201
331.5	0.8217	0.1783
334.7	0.8000	0.2000
341.5	0.7435	0.2565
350.9	0.6263	0.3737
356.9	0.4979	0.5021
357.0	0.4906	0.5094
360.1	0.3953	0.6047
362.7	0.3046	0.6954

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the eutectic point occurred at $x_1 = 0.0439$ and T/K $= 290.6$.

Auxiliary Information

Method/Apparatus/Procedure:
Heating circulating bath and platinum resistance temperature probe. Synthetic mixtures of known compositions were prepared by mass. Samples were slowly heated in a temperature bath, and the temperature at which the last amount of solid solute dissolved was measured. The temperature obtained was taken to represent the saturation point for the mixture being studied.

Source and Purity of Chemicals:
(1) 98.0%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.0%, Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[43]L. F. Ramirez-Verduzco, A. Rojas-Aguilar, J. A. De los Reyes, J. A. Munoz-Arroyo, and F. Murrieta-Guevara, J. Chem. Eng. Data **52**, 2212 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
309.3	0.9504	0.0496
321.1	0.9129	0.0871
328.8	0.8709	0.1291
335.6	0.8011	0.1989
349.6	0.5076	0.4924
353.5	0.4070	0.5930

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Heating circulating bath and platinum resistance temperature probe. Synthetic mixtures of known compositions were prepared by mass. Samples were slowly heated in a temperature bath, and the temperature at which the last amount of solid solute dissolved was measured. The temperature obtained was taken to represent the saturation point for the mixture being studied.

Source and Purity of Chemicals:
(1) 98.0%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±0.0005.

7.3. Dibenzothiophene solubility data in esters

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Dihydro-2(3*H*)-furanone (γ-butyrolactone); $C_4H_6O_2$; [96-48-0]	[43]L. F. Ramirez-Verduzco, A. Rojas-Aguilar, J. A. De los Reyes, J. A. Munoz-Arroyo, and F. Murrieta-Guevara, J. Chem. Eng. Data **52**, 2212 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
281.3	0.9401	0.0599
289.7	0.9238	0.0762
300.1	0.8953	0.1047
307.9	0.8652	0.1348
314.6	0.8332	0.1668
320.2	0.7989	0.2011
325.2	0.7624	0.2376
329.4	0.7257	0.2743
337.6	0.6370	0.3630
344.6	0.5365	0.4635
351.5	0.4167	0.5833
354.8	0.3497	0.6503
362.4	0.1924	0.8076

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Heating circulating bath and platinum resistance temperature probe. Synthetic mixtures of known compositions were prepared by mass. Samples were slowly heated in a temperature bath, and the temperature at which the last amount of solid solute dissolved was measured. The temperature obtained was taken to represent the saturation point for the mixture being studied.

Source and Purity of Chemicals:
(1) 98.0%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.0%, Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±0.0005.

7.4. Dibenzothiophene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[43]L. F. Ramirez-Verduzco, A. Rojas-Aguilar, J. A. De los Reyes, J. A. Munoz-Arroyo, and F. Murrieta-Guevara, J. Chem. Eng. Data **52**, 2212 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.7	0.9801	0.0199
323.1	0.9478	0.0522
332.0	0.8979	0.1021
338.1	0.8014	0.1986
341.8	0.6908	0.3092
344.8	0.6044	0.3956
347.1	0.5396	0.4604

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Heating circulating bath and platinum resistance temperature probe. Synthetic mixtures of known compositions were prepared by mass. Samples were slowly heated in a temperature bath, and the temperature at which the last amount of solid solute dissolved was measured. The temperature obtained was taken to represent the saturation point for the mixture being studied.

Source and Purity of Chemicals:
(1) 98.0%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, Fermont Company, was used as received.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
253.2	1.0000	0.0000
252.9	0.9892	0.0108
252.1	0.9790	0.0210
251.3	0.9673	0.0327
250.6	0.9463	0.0537
250.9	0.9250	0.0750
256.5	0.9140	0.0860
269.0	0.8912	0.1088
289.7	0.8299	0.1701
300.7	0.7848	0.2152
318.0	0.6875	0.3175
331.9	0.5729	0.4271
341.4	0.4727	0.5273
347.8	0.3979	0.6021
355.3	0.2926	0.7074
361.4	0.1906	0.8094
366.9	0.0990	0.9010
369.0	0.0498	0.9502
371.8	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 249.6$ and eutectic composition of $x_1 = 0.073$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002. mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Purest grade, Merck-Schuchardt, was distilled under reduced pressure and dried over molecular sieves to produce a sample of 99.9% purity (mass percent).

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
248.5	1.0000	0.0000
247.3	0.9798	0.0202
246.3	0.9648	0.0352
245.7	0.9463	0.0537
244.7	0.9195	0.0805
248.1	0.8797	0.1203
276.6	0.8390	0.1610
284.8	0.7940	0.2060
298.2	0.7393	0.2607
309.2	0.6871	0.3129
318.0	0.6389	0.3611
325.9	0.5859	0.4141
330.5	0.5525	0.4475
336.6	0.4936	0.5064
342.1	0.4444	0.5556
347.3	0.3851	0.6149
353.5	0.2968	0.7032
359.3	0.2133	0.7867
366.3	0.0977	0.9023
371.8	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 242.7$ and eutectic composition of $x_1 = 0.111$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Technical Grade, BASF, Federal Republic of Germany, was purified by treatment with a 2% solution of potassium permanganate, and then distilled under reduced pressure to collect the distillate having 99.8% purity (mass percent). The purified sample was dried over molecular sieves.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Hexahydro-1-methyl-2*H*-azepin-2-one (*N*-Methyl-ε-caprolactam); $C_7H_{13}NO$; [2556-73-2]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
279.6	1.0000	0.0000
282.3	0.7978	0.2022
296.7	0.7494	0.2506
305.4	0.7023	0.2977
313.8	0.6489	0.3511
321.6	0.5982	0.4018
328.4	0.5493	0.4507
335.5	0.4948	0.5052
345.9	0.3917	0.6083
354.3	0.2859	0.7141
360.4	0.1977	0.8023
365.6	0.1091	0.8909
371.8	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperatures at which the solid completely dissolved were recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Technical Grade, Leuna Werke, Federal Republic of Germany, was purified by super-rectification and then dried over molecular sieves to give a sample having a purity of 99.9% by mass.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

8. Solubility of Fluoranthene in Organic Solvents

8.1. Critical evaluation of experimental solubility data

Vol. 59 in the IUPAC Solubility Data Series[3] contained experimental solubility data for fluoranthene in one cycloalkane (cyclohexane), in one aromatic hydrocarbon (methylbenzene), in one cyclic ether (1,4-dioxane), in one chlorinated alkane (tetrachloromethane) and chlorinated aromatic hydrocarbon (chlorobenzene), in three alkanols (methanol, ethanol and 1-octanol) and one substituted phenol (1-hydroxy-2-methylbenzene), in one alkanone (propanone), and in three miscellaneous organic solvents (pyridine, nitrobenzene and dimethylsulfoxide). For each of the aforementioned systems there was only a single measurement made near 298.15 K. The volume also included phase diagram information for binary fluoranthene + benzene, fluoranthene + 1,2,4,5-tetramethylbenzene, fluoranthene + naphthalene, fluoranthene + 2-methylnaphthalene, fluoranthene + 2,7-dimethylnaphthalene, fluoranthene + fluorene, fluoranthene + anthracene, fluoranthene + phenanthrene, fluoranthene + acenaphthene, fluoranthene + chrysene, fluoranthene + 1,4-dinitrobenzene, fluoranthene + 1,4-dinitrobenzene, fluoranthene + 1,3,5-trinitrobenzene, fluoranthene + 1,2,3,5-tetranitrobenzene, fluoranthene + 2,3-nitromethylbenzene, fluoranthene + 2,4-dinitrophenol, fluoranthene + 2,4,6-trinitromethylbenzene, fluoranthene + 2,4,6-trinitromethoxybenzene, fluoranthene + 2,4,6-trinitroaniline, fluoranthene + 2-chloro-1,3,5-trinitrobenzene, and fluoranthene + 3-methyl-2,4,6-trinitrophenol mixtures. Solubility data contained in Vol. 59 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for fluoranthene.

There have been three studies that reported solubility data for fluoranthene dissolved in organic solvents after Vol. 59 was published in 1995. Hernández and Acree[44] determined the solubility of fluoranthene in 36 different organic solvents containing ether-, hydroxy-, ester-, chloro-, methyl-, and *tert*-butyl functional groups. Roy *et al.*[45] later measured fluoranthene solubilities in benzene, methylbenzene, trichloromethane, tetrachloromethane, 1,2-dichloroethane, 1-chlorohexane, 1,2-ethanediol, 2,2,2-trifluoroethanol, ethanenitrile, *N*,*N*-dimethylformamide, and *N*,*N*-dimethylformamide. The experimental measurements were performed at the single temperature of 298.15 K and used to test the limitations and applications of predictive expressions based on Mobile Order theory. For the majority of the solvents studied by Hernández and Acree[44] and by Roy *et al.*[45] there is only the single experimental value, and it is not possible to perform a critical evaluation on most of the published data.

There exist independent experimental values for the solubility of fluoranthene in both methanol [$c_1 = 0.0704$ mol dm^{-3} at 296.15 K (Ref. 46)] and 1-octanol [$c_1 = 0.1726$ mol dm^{-3} at 298.15 K (Ref. 47) and $c_1 = 0.198$ mol dm^{-3} at 296.15 K (Ref. 46)] measured at or near 298.15 K in Vol. 59 of the Solubility Data Series.[3] The experimental solubility data determined by Hernández and Acree,[44] when converted to molar solubilities ($c_1 = 0.0557$ mol dm^{-3} for methanol and $c_1 = 0.198$ mol dm^{-3} for 1-octanol), are in reasonably good agreement with the earlier published values. McLauglin and Zainal[11] conducted fluoranthene solubility measurements in cyclohexane from 301.8 to 344.2 K. The dataset is in Vol. 59.[3] Analysis of the measured fluoranthene mole fraction solubilities using Eq. (3) gave the following mathematical correlation:

$$\ln x_1 = 10.549 - \frac{4127.4}{T} + 3.544 \ln T. \tag{8}$$

Equation (8) provides a reasonably accurate mathematical description of the solubility behavior of fluoranthene in cyclohexane. Differences between the experimental data and values back-calculated using Eq. (8) were on the order of 11% or less. Equation (8) gives an extrapolated value of $x_1 = 0.01502$ for the mole fraction solubility of fluoranthene in cyclohexane, which is less than the value of $x_1 = 0.01807$ that was reported by Hernández and Acree.[44] Differences in chemical purities and experimental methodologies were the likely causes of the deviations noted in the published solubility data for fluoranthene dissolved in methanol, 1-octanol and cyclohexane noted above.

The experimental solubility data for fluoranthene in the different organic solvents are given in Secs. 8.2–8.8.

8.2. Fluoranthene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Hexane; C_6H_{14}; [110-54-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9852	0.01476

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Heptane; C_7H_{16}; [142-82-5]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9813	0.01870

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Octane; C_8H_{18}; [111-65-9]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9774	0.02260

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Nonane; C_9H_{20}; [111-84-2]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9736	0.02642

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9698	0.03015

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9495	0.05046

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Octacosane; $C_{28}H_{58}$; [630-02-4]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
333.91	1.0000	0.0000
333.75	0.8993	0.1007
333.65	0.7978	0.2022
333.21	0.7001	0.2999
349.40	0.5979	0.4021
362.55	0.5001	0.4999
370.34	0.3976	0.6024
372.26	0.3350	0.6650
373.09	0.3001	0.6999
377.28	0.2004	0.7996
379.29	0.1002	0.8998
382.35	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of fluoranthene and octacosane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 329.7$ and eutectic mole fraction of fluoranthene of $x_1 = 0.270$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
$T/\mathrm{K} = 298.15$	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9819	0.01807

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
$T/\mathrm{K} = 298.15$	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9782	0.02179

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[44] C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9699	0.03011

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[44] C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9884	0.01162

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]	[44] C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9752	0.02482

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^a	x_1^b
339.75	0.7944	0.2056
354.45	0.6928	0.3072
362.85	0.5987	0.4013
369.05	0.4970	0.5030
372.95	0.4000	0.6000
374.65	0.3505	0.6495
375.75	0.2998	0.7002
377.60	0.2008	0.7992
378.35	0.1502	0.8498
378.95	0.1019	0.8981
380.05	0.0510	0.9490

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of fluoranthene and squalane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 234.1$ and eutectic mole fraction of fluoranthene of $x_1 = 0.006$.

Auxiliary Information

Method/Apparatus/Procedure:
Simple thermal analysis device constructed in the authors' laboratory, and a high precision platinum-resistance thermometer.
The phase diagram was determined using a simple thermal device. A sample of known composition was placed in a thermostatted glass tube, melted and then slowly cooled at a rate of about 1 K/min. The temperature of the sample was measured with a high precision platinum-resistance thermometer. The crystallization temperature was obtained from a plot of the cooling curve versus time. Each measurement was repeated three times.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

8.3. Fluoranthene solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Benzene; C_6H_6; [71-43-2]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.8789	0.1211

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Methylbenzene; C_7H_8; [108-88-8]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8840	0.1160

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

8.4. Fluoranthene solubility data in esters

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9141	0.08589

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8894	0.1106

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

8.5. Fluoranthene solubility data in ethers

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9482	0.05177

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9524	0.04755

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

8.6. Fluoranthene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8574	0.1426

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, was shaken several times with an aqueous sodium hydroxide solution and then with distilled water to remove the ethanol stabilizer. The resulting solution was dried over both anhydrous calcium chloride and molecular sieves, and then distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9184	0.08157

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8732	0.1268

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8867	0.1133

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5+%, HPLC Grade, Sigma-Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8685	0.1315

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8633	0.1367

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8841	0.1159

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

8.7. Fluoranthene solubility data in alcohols

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Methanol; CH_4O; [67-56-1]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9977	0.002267

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Ethanol; C_2H_6O; [64-17-5]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9946	0.00544

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9933	0.00670

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Propanol; C_3H_8O; [67-63-0]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9952	0.00475

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9900	0.00996

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9930	0.00702

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9950	0.00495

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9855	0.01446

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9898	0.01021

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9914	0.00862

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9903	0.00970

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9801	0.01986

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9883	0.01172

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9905	0.00948[d]

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.
[d] There is a typographical error in the published mole fraction solubility. The correct value is 0.00948.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9748	0.02524

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9687	0.03125

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9822	0.01782

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]	[44]C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9823	0.01772

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[45]L. E. Roy, C. E. Hernández and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9992	0.000750

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9992	0.000772

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

8.8. Fluoranthene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9868	0.01315

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8203	0.1797

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.7630	0.2370

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 357 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

9. Solubility of Fluorene in Organic Solvents

9.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained experimental solubility data for fluorene dissolved in two cycloalkanes (cyclohexane and decahydronaphthalene), in four aromatic hydrocarbons (benzene, methylbenzene, 1,4-dimethylbenzene, and 1,2,3,4-tetrahydronaphalene), in one chlorinated alkane (tetrachloromethane) and one chlorinated benzene (chlorobenzene), in three alkanols (methanol, ethanol, and 1-octanol), and in four miscellaneous organic solvents (nitrobenzene, pyridine, aniline, and thiophene). Except for the fluorene + methanol system, each data set contained mole fraction solubilities measured at several temperatures. The volume also included phase diagram information for binary fluorene + benzene, fluorene + ethylbenzene, fluorene + 1,3-dimethylbenzene, fluorene + 1,2,4,5-tetramethylbenzene, fluorene + naphthalene, fluorene + 2-methylnaphthalene, fluorene + 2,7-dimethylnaphthalene, fluorene + fluoranthene, fluorene + acenaphthene, fluorene + chrysene, fluorene + 1,2-dinitrobenzene, fluorene + 1,3-dinitrobenzene, fluorene + 1,4-dinitrobenzene, fluorene + 1,3,5-trinitrobenzene, fluorene + 1,2,3,5-tetranitrobenzene, fluorene + 2,4-dinitromethylbenzene, fluorene + 2,4,6-trinitromethylbenzene, fluorene + 2,4-dinitrophenol, fluorene + 2,4,6-trinitrophenol, and fluorene + 6-methyl-2,3,4-trinitrophenol mixtures. Solubility data contained in Vol. 59 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for fluorene.

There have been several studies that reported solubility data for fluorene in organic solvents after Vol. 59 was published in 1995. Monárrez *et al.*[48] investigated the solubility of fluorene in 13 primary, four secondary, and two tertiary alcohols. In a followup study, Stovall *et al.*[49] measured the solubility of fluorene in several alkane, dialkyl ether and alkanenitrile solvents. Experimental results from both studies were used to test the applications and limitations of the Abraham solvation parameter model in regards to solubility predictions. The authors measured the solubility at only 298.15 K, and except for five alkanol solvents there are no independent experimental measurements to compare the numerical values against.

Two research groups studied the solubility behavior of fluorene as a function of temperature. Zou *et al.*[50] examined the solubility of fluorene in methylbenzene, ethanol, 2-propanol, and 1-butanol at ten different temperatures using a synthetic method with laser monitoring. Han and Wang[51] later measured the solubility of fluorene in benzene, trichloromethane, propanone, 1-propanol, 2-methyl-1-propanol, and methylbenzene from 283 to 323 K also using a laser monitoring method. The solubility measurements in the alkanol solvents from these two studies can be compared to the values reported by Monárrez *et al.*[48] Reasonably good agreement is found in the case of ethanol ($x_1 = 0.00743$ in Ref. 48 versus $x_1 = 0.00802$ in Ref. 50), 1-propanol ($x_1 = 0.01232$ in Ref. 48 versus $x_1 = 0.01339$ in Ref. 51), and 2-methyl-1-propanol ($x_1 = 0.01006$ in Ref. 48 versus $x_1 = 0.00902$ in Ref. 50). Much larger deviations were observed in the case of 2-propanol ($x_1 = 0.00949$ in Ref. 48 versus $x_1 = 0.00423$ in Ref. 50) and 1-butanol ($x_1 = 0.01689$ in Ref. 48 versus $x_1 = 0.01030$ in Ref. 50). No explanation is given for the larger deviations noted for the latter two alkanol solvents.

The internal consistency of the Zou *et al.*[50] and Han and Wang[51] datasets were assessed by curve-fitting the measured mole fraction solubility to Eq. (3). The numerical values of the equation coefficients (A, B, and C) are given in Table 3, along with the MRD calculated according to Eq. (7). Examination of the numerical entries in the last column of Table 3 reveals that the largest mean relative percent deviation between the back-calculated values based on Eq. (3) and experimental data is only 7.1%. Deviations for the other systems are much less and are often even less than the experimental uncertainties in the measured values. Results of the mathematical representation analyses indicate that the experimental data for all ten fluorene–organic solvent systems are internally consistent. It is further noted that the two sets of solubility data for fluorene in methylbenzene are in good agreement with each other, with the calculated average absolute relative deviation being less than 2%.

TABLE 3. Parameters of the Apelblat equation for describing the solubility of fluorene in various organic solvents

Solvent	A	B	C	MRD (%)
Methylbenzene[a]	−103.83	1180.4	17.162	1.2
Ethanol[a]	−102.96	1448.2	16.369	<0.1
2-Propanol[a]	−68.045	−1896.3	12.096	<0.1
1-Butanol[a]	−88.212	508.8	14.390	0.3
Benzene[b]	−97.752	2365.2	15.401	1.2
Trichloromethane[b]	−64.383	801.3	10.474	0.7
Propanone[b]	−64.406	487.2	10.545	2.2
1-Butanol[b]	−65.649	305.9	10.586	2.8
2-Methyl-1-propanol[b]	−96.548	710.9	10.709	7.1
Methylbenzene[b]	−101.009	1132.4	16.702	3.5

[a] Numerical values of the coefficients and the percent mean relative deviations were taken from Zou *et al.*[50]

[b] Numerical values of the coefficients and the percent mean relative deviations were taken from Han and Wang.[51]

Lisicki and Jamróz[35] reported solid-liquid equilibria data for binary mixtures containing fluorene with *N*,*N*-dimethylacetamide, 1-methyl-2-pyrrolidone and hexahydro-1-methyl-2*H*-azepin-2-one (also called *N*-methyl-ε-caprolactam). The fluorene + *N*,*N*-dimethylformamide and anthracene + 1-methyl-2-pyrrolidone systems both exhibited simple eutectic behavior. The published experimental liquidus curves for the latter three fluorene systems did not indicate any outlier data points.

The experimental solubility data for fluorene dissolved in the different organic solvents are given in Secs. 9.2–9.9.

9.2. Fluorene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Hexane; C_6H_{14}; [110-54-3]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9696	0.03041

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Heptane; C_7H_{16}; [142-82-5]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9659	0.03406

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Octane; C_8H_{18}; [111-65-9]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9625	0.03750

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4]
(2) Nonane; C_9H_{20}; [111-84-2]

Original Measurements:
[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9573	0.04269

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4]
(2) Decane; $C_{10}H_{22}$; [124-18-5]

Original Measurements:
[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9533	0.04669

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4]
(2) Undecane; $C_{11}H_{24}$; [1120-21-4]

Original Measurements:
[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9495	0.05048

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Dodecane; $C_{12}H_{26}$; [112-40-3]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9470	0.05302

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9322	0.06781

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Octacosane; $C_{28}H_{58}$; [630-02-4]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
333.91	1.0000	0.0000
332.95	0.8981	0.1019
332.69	0.7881	0.2119
332.19	0.7540	0.2460
340.80	0.6916	0.3084
352.41	0.6011	0.3989
359.00	0.4935	0.5065
365.60	0.4002	0.5998
370.67	0.2997	0.7003
377.23	0.2002	0.7998
382.34	0.1001	0.8999
387.25	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of fluorene and octacosane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 332.3$ and eutectic mole fraction of fluorene of $x_1 = 0.226$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9623	0.03768

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9602	0.03975

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

Variables:	Prepared by:
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9502	0.04977

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Lancaster Synthesis, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

Variables:	Prepared by:
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9746	0.02537

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.7%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

Variables:	Prepared by:
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9561	0.04385

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
324.35	0.7999	0.2001
340.45	0.6983	0.3017
351.85	0.5992	0.4008
360.95	0.5014	0.4986
365.15	0.4504	0.5496
368.75	0.3899	0.6101
371.25	0.3502	0.6498
373.85	0.2968	0.7032
376.35	0.2506	0.7494
377.95	0.2024	0.7976
380.05	0.1514	0.8486
381.65	0.1000	0.9000
383.85	0.0540	0.9460

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of fluorene and squalane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 234.0$ and eutectic mole fraction of fluorene of $x_1 = 0.01$.

Auxiliary Information

Method/Apparatus/Procedure:
Simple thermal analysis device constructed in the authors' laboratory, and a high precision platinum-resistance thermometer.
Phase diagram was determined using a simple thermal device. A sample of known composition was placed in a thermostatted glass tube, melted and then slowly cooled at a rate of about 1 K/min. The temperature of the sample was measured with a high precision platinum-resistance thermometer. The crystallization temperature was obtained from a plot of the cooling curve versus time. Each measurement was repeated three times.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

9.3. Fluorene solubility data in aromatic hydrocarbons

Components:`	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Benzene; C_6H_6; [71-43-2]	[51]Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.00	0.9117	0.08832
288.00	0.9018	0.09824
293.00	0.8909	0.1091
298.00	0.8743	0.1257
303.20	0.8568	0.1432
308.00	0.8416	0.1584
313.00	0.8165	0.1835
318.00	0.7909	0.2091
323.00	0.7654	0.2346

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which the last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) 99+%, Chemical source and purification method were not given.
(2) 99.8+%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Methylbenzene; C_7H_8; [108-88-8]	[51]Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.00	0.9370	0.06295
288.00	0.9191	0.08088
293.00	0.9033	0.09674
298.00	0.8761	0.1239
303.20	0.8475	0.1525
308.00	0.8048	0.1952
313.00	0.7503	0.2497
318.00	0.7001	0.2999
323.00	0.6304	0.3696

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which the last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) 99+%, Chemical source and purification method were not given.
(2) 99.8+%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Methylbenzene; C_7H_8; [108-88-8]	[50]Z. Zou, L. Dang, P. Liu, and H. Wei, J. Chem. Eng. Data **52**, 1501 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.27	0.9366	0.06341
288.77	0.9181	0.08185
293.72	0.8981	0.1019
298.89	0.8705	0.1295
303.17	0.8455	0.1545
308.81	0.7995	0.2005
313.17	0.7471	0.2521
319.27	0.6923	0.3077
324.95	0.6329	0.3671

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

9.4. Fluorene solubility data in esters

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9333	0.06667

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

9.5. Fluorene solubility data in ethers

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9468	0.05324

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9277	0.07226

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

9.6. Fluorene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[51]Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
283.00	0.9107	0.08928
288.00	0.8984	0.1016
293.00	0.8856	0.1144
298.00	0.8682	0.1318
303.20	0.8474	0.1526
308.00	0.8269	0.1731
313.00	0.8048	0.1952
318.00	0.7801	0.2199
323.00	0.7503	0.2497

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) 99+%, Chemical source and purification method were not given.
(2) 99.8+%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

9.7. Fluorene solubility data in alcohols

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Methanol; CH_4O; [67-56-1]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$	x_2	x_1
1.0000	0.9955	0.00449

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Ethanol; C_2H_6O; [64-17-5]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$	x_2	x_1
1.0000	0.9926	0.00743

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Ethanol; C_2H_6O; [64-17-5]	[50]Z. Zou, L. Dang, P. Liu, and H. Wei, J. Chem. Eng. Data **52**, 1501 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.98	0.9963	0.00372
283.99	0.9954	0.00455
289.01	0.9945	0.00554
294.08	0.9933	0.00668
298.35	0.9920	0.00802
303.36	0.9903	0.00973
308.77	0.9881	0.01185
313.17	0.9861	0.01387
319.27	0.9823	0.01766
324.95	0.9784	0.02161

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components: (1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Propanol; C_3H_8O; [71-23-8]	**Original Measurements:** [48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9877	0.01232

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Propanol; C_3H_8O; [71-23-8]	**Original Measurements:** [51]Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.00	0.9918	0.00817
288.00	0.9910	0.00903
293.00	0.9985	0.01154
298.40	0.9866	0.01339
302.20	0.9837	0.01631
308.00	0.9812	0.01882
313.00	0.9785	0.02151
318.00	0.9752	0.02483
323.00	0.9711	0.02890

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) 99+%, Chemical source and purification method were not given.
(2) 99.8+%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Propanol; C_3H_8O; [67-63-0]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9905	0.00949

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Propanol; C_3H_8O; [67-63-0]	[50]Z. Zou, L. Dang, P. Liu, and H. Wei, J. Chem. Eng. Data **52**, 1501 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
288.28	0.9978	0.00221
293.69	0.9969	0.00313
299.50	0.9955	0.00453
303.17	0.9943	0.00565
309.06	0.9918	0.00820
313.78	0.9895	0.01047
318.24	0.9864	0.01355
323.17	0.9821	0.01787
328.25	0.9763	0.02368
333.45	0.9686	0.03136

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200.

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9831	0.01686

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4]	[50]Z. Zou, L. Dang, P. Liu, and H. Wei,
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	J. Chem. Eng. Data **52**, 1501 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
284.27	0.9941	0.00590
288.82	0.9928	0.00724
293.76	0.9909	0.00906
298.88	0.9887	0.01130
304.06	0.9861	0.01390
308.28	0.9832	0.01679
313.93	0.9788	0.02122
318.16	0.9749	0.02510
323.16	0.9696	0.03038
328.25	0.9630	0.03703
333.35	0.9542	0.04578
338.35	0.9442	0.05584

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated bath, thermometer.
Very little experimental details were provided. Solubilities were determined by a synthetic method. Known masses of solute and solvent were placed in a dissolving flask. The solute and solvent mixture was stirred with a magnetic stirrer. Small amounts of solute were added at predetermined intervals until no more solid would dissolve. The point at which no more solid would dissolve was taken to be the point of solid-liquid equilibrium. The paper did not specify how the disappearance of the solid was monitored; however, the papers that the authors referenced for the experimental method used a laser monitoring method.

Source and Purity of Chemicals:
(1) 99.5%, Chemical source and purification method were not given.
(2) 99.8%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200.

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4]	[48]C. I. Monárrez, W. E. Acree, Jr., and
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9879	0.01206

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4]	[48]C. I. Monárrez, W. E. Acree, Jr., and
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9899	0.01006

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[51]Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^a	x_1^b
283.00	0.9957	0.00425
288.00	0.9946	0.00544
293.00	0.9931	0.00691
298.40	0.9910	0.00902
303.20	0.9879	0.01212
308.00	0.9844	0.01563
313.00	0.9808	0.01924
318.00	0.9770	0.02296
323.00	0.9733	0.02668

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) 99+%, Chemical source and purification method were not given.
(2) 99.8+%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9898	0.01016

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9771	0.02290

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9837	0.01634

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9816	0.01842

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9854	0.01461

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9815	0.01854

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9724	0.02757

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9803	0.01973

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9832	0.01676

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9650	0.03503

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9612	0.03884

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9721	0.02794

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[48]C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9533	0.04669

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

9.8. Fluorene solubility data in ketones

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Propanone; C_3H_6O; [67-64-1]	[51]Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.00	0.9555	0.04448
288.00	0.9510	0.04896
293.00	0.9442	0.05577
298.00	0.9313	0.06872
303.10	0.9207	0.07931
308.20	0.9093	0.09074
313.00	0.8962	0.1038
318.00	0.8802	0.1198
323.00	0.8602	0.1398

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) 99+%, Chemical source and purification method were not given.
(2) 99.8+%, Analytical Reagent Grade, Tianjin Kewei Company, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: within 0.0200 (relative uncertainty).

9.9. Fluorene solubility data in miscellaneous organic solvents

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Propanenitrile; C_3H_5N; [107-12-0]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9418	0.05815

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Butanenitrile; C_4H_7N; [109-74-0]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9145	0.08548

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Hexanedinitrile; $C_6H_8N_2$; [111-69-3]	[49]D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9541	0.04589

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) *N,N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
253.2	1.0000	0.0000
252.9	0.9898	0.0102
252.3	0.9792	0.0208
251.6	0.9698	0.0302
250.7	0.9599	0.0401
254.0	0.9500	0.0500
272.7	0.9180	0.0820
285.7	0.8913	0.1087
304.8	0.8298	0.1702
314.7	0.7839	0.2161
332.7	0.6739	0.3261
342.8	0.5938	0.4062
353.8	0.4822	0.5178
360.1	0.4158	0.5842
371.6	0.2972	0.7028
375.5	0.2133	0.7867
379.9	0.1459	0.8541
385.1	0.0481	0.9519
387.7	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of T/K = 250.1 and eutectic composition of $x_1 = 0.046$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.
(2) Purest grade, Merck-Schuchardt, was distilled under reduced pressure and dried over molecular sieves to produce a sample of 99.9% purity (mass percent).

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
248.5	1.0000	0.0000
247.7	0.9781	0.0219
246.8	0.9503	0.0497
246.0	0.9338	0.0662
245.6	0.9241	0.0759
249.1	0.9139	0.0861
262.0	0.8933	0.1067
274.4	0.8724	0.1276
283.0	0.8509	0.1491
293.7	0.8201	0.1799
295.4	0.8139	0.1861
303.7	0.7845	0.2155
322.6	0.6936	0.3064
339.0	0.5885	0.4115
351.7	0.4840	0.5160
356.3	0.4398	0.5602
358.8	0.4130	0.5870
363.3	0.3602	0.6398
366.2	0.3263	0.6737
374.1	0.2295	0.7705
374.7	0.2216	0.7784
383.8	0.0793	0.9207
384.9	0.0624	0.9376
387.7	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 245.3$ and eutectic composition of $x_1 = 0.082$.

Auxiliary Information

Method/Apparatus/Procedure:

Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:

(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.

(2) Technical Grade, BASF, Federal Republic of Germany, was purified by treatment with a 2% solution of potassium permanganate, and then distilled under reduced pressure to collect the distillate having 99.8% purity (mass percent). The purified sample was dried over molecular sieves.

Estimated Error:

Temperature: ±0.2 K (estimated by compiler).

x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Fluorene; $C_{13}H_{10}$; [92-52-4] (2) Hexahydro-1-methyl-2*H*-azepin-2-one (*N*-Methyl-ε-caprolactam); $C_7H_{13}NO$; [2556-73-2]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
279.6	1.0000	0.0000
304.3	0.8049	0.1951
315.7	0.7463	0.2537
324.3	0.6988	0.3012
332.3	0.6499	0.3501
339.2	0.5970	0.4030
347.5	0.5290	0.4710
352.0	0.4911	0.5089
356.3	0.4508	0.5492
361.3	0.4004	0.5996
365.9	0.3480	0.6520
370.1	0.2964	0.7036
377.7	0.1978	0.8022
383.5	0.0999	0.9001
387.7	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down, and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:

(1) 98%, Merck-Schuchardt, Federal Republic of Germany, was recrystallized twice from ethanol in the presence of activated carbon, and then recrystallized from methylbenzene.

(2) Technical Grade, Leuna Werke, Federal Republic of Germany, was purified by super-rectification and then dried over molecular sieves to give a sample having a purity of 99.9% by mass.

Estimated Error:

Temperature: ±0.2 K (estimated by compiler).

x_1: ±0.0002.

10. Solubility of Naphthalene in Organic Solvents

10.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained experimental solubility data for naphthalene dissolved in five linear alkanes (hexane, heptane, octane, hexadecane, and octadecane) and eight cycloalkanes (cyclohexane, methylcyclohexane, *cis*-1,2-dimethyl-cyclohexane, *trans*-1,2-dimethylcyclohexane, *cis*-1,3-dimethylcyclohexane, *cis*-1,4-dimethylcylcohexane, *trans*-1,4-dimethylcyclohexane, and decahydronaphthalene), in five aromatic hydrocarbons (benzene, methylbenzene, ethylbenzene, 1,2,3,4-tetrahydronaphthalene, and 4-isopropyl-1-methylbenzene), in five esters (furfuryl acetate, methyl 2-furoate, ethyl 2-furoate, propyl 2-furoate, and butyl 2-furoate), in four dialkyl ethers (1,1′-oxybisethane, 1,1′-oxybisbutane, 1-ethoxypropane, and 2-ethoxypropane), and three cyclic ethers (2,2-dimethyloxetane, 3,3-dimethyloxetane, and tetrahydrofuran), in eight halogenated alkanes (dichloromethane, trichloromethane, tetrachloromethane, diiodomethane, 1,1-dibromoethane, 1,2-dibromoethane, 1,1-dichloroethane, 1,2-dichloroethane), one chloroalkene (trichloroethene) and two halogenated benzenes (chlorobenzene and hexafluorobenzene), in 14 alkanols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 1-hexanol, 1-octanol, cyclohexanol, methylcyclohexanol, and furfuryl alcohol), in one alkanone (propanone) and in seven miscellaneous organic solvents (carbon disulfide, nitrobenzene, aniline, thiophene, pyridine, perfluorodibutyl ether, and perfluorotripropylamine). The volume also included phase diagram information for binary naphthalene + benzene, naphthalene + methylbenzene, naphthalene + ethylbenzene, naphthalene + 1,2-dimethylbenzene, naphthalene + 1,3-dimethylbenzene, naphthalene + 1,4-dimethylbenzene, naphthalene + biphenyl, naphthalene + 1,2-diphenylethane, naphthalene + indene, naphthalene + fluoranthene, naphthalene + fluorene, naphthalene + chrysene, naphthalene + pyrene and naphthalene + acenaphthene, naphthalene + 1,4-dichlorobenzene, naphthalene + octafluoronaphthalene, naphthalene + 1,2-benzenediol, naphthalene + 1,3-benzenediol, naphthalene + 1,4-benzenediol, naphthalene + 2-nitrobenzaldehyde, naphthalene + 3-nitrobenzaldehyde, naphthalene + 4-nitrobenzaldehyde, naphthalene + 1-chloro-3-nitrobenzene, naphthalene + 1-chloro-4-nitrobenzene, naphthalene + 2,4-dinitroaniline, naphthalene + 3,5-dinitrobenzoic acid, naphthalene + 1,3,5-trimethyl-2,4,6-trinitrobenzene, naphthalene + 4-nitro-1-methylbenzene, naphthalene + 1,3-dinitrobenzene, naphthalene + 1,3,5-trinitrobenzene, naphthalene + 2-nitrophenol, naphthalene + 4-nitrophenol, naphthalene + 2,4-dinitro-1-methylbenzene, naphthalene + 2,4-dinitrophenol, naphthalene + 2,4,6-trinitrophenol, and naphthalene + isoquinoline. Solubility data contained in Vol. 59 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for naphthalene.

There have been several studies that reported solubility data for naphthalene in organic solvents after Vol. 59 was published in 1995. Numerous research groups have studied the solubility behavior of naphthalene as a function of temperature. Cui *et al.*[52] examined the solubility of naphthalene in heptanes, methylbenzene, ethanol, 1-butanol, propanone, and in a mixture of dimethylbenzene isomers (13.3% 1,2-dimethylbenzene, 66.4% 1,3-dimethylbenzene, and 20.3% 1,4-dimethylbenzene) using a dynamic method with laser detection system. Plots of naphthalene mole fraction solubilities versus temperature given in the paper fell on smooth curves. As part of the study the authors determined curve-fit equation coefficients for mathematical describing the measured mole fraction solubilities with the Apelblat (see Eq. (3)) and Buchowski λh (see Eq. (4)) models. The calculated equation coefficients are given in Tables 4 and 5, respectively. Average deviations between the experimental data and calculated values based on the Apelblat and Buchowski λh models were on the order of 4.6% and 8.1%, respectively. Li *et al.*[53] studied the solubility of naphthalene in ethyl ethanoate, 2-methylpropyl ethanoate, tetrahydrofuran, butanoic acid, *N*,*N*-dimethylformamide, and 2-methyl-2-pyrrolidone between 278 and 328 K. The calculated coefficients for the Apelblat mathematical representation are given in Table 4. The six datasets are judged to be internally consistent, with mean relative deviations between the observed data and values calculated based on Apelblat model being less than 7.5%. Both research groups studied the solubility of naphthalene in propanone. There is less than a 5% difference between the two datasets.

Kotula and Marciniak[13] published solubility data for naphthalene in four chlorinated alkanes (trichloromethane, tetrachloromethane, 1,1-dichloroethane, and 1,2-dichloroethane) and two chlorinated alkenes (trichloroethene and tetrachloroethene) from 290 to 325 K. The internal consistency of the chloroalkane and chloroalkene datasets of measured acenaphthene solubilities were assessed by curve-fitting the measured the mole fraction solubility data to Eq. (3). The numerical values of the equation coefficients (A, B, and C) are given in Table 4 along with the respective mean relative deviations. Examination of the numerical entries in the last column of the table reveals that the Apelblat equation provides a very good description of the solubility behavior in the four chloroalkane and two chloroalkene solvents with the average mean relative deviations being on the order of 0.4% or less.

Published studies[15,39,42,54–58] have also included phase diagrams for binary naphthalene mixtures containing a variety of different organic compounds, including saturated hydrocarbons (eicosane, pentacosane, octacosane, *trans*-decahydronaphthalene, and *cis*-decahydronaphthalene), polycyclic aromatic hydrocarbons (biphenyl and phenanthrene) and chlorinated benzenes (1,2-dichlorobenzene, 1,3-dichlorobenzene, and 1,4-dichlorobenzene). Phase diagrams and discussions given in the papers did not suggest any inconsistencies in the individual datasets.

The experimental solubility data for naphthalene dissolved in the different organic solvents are given in Secs. 10.2–10.9.

TABLE 4. Parameters of the Apelblat equation for describing the solubility of naphthalene in various organic solvents

Solvent	*A*	*B*	*C*	MRD (%)
Heptane[a]	−127.81	195.1	20.824	
Methylbenzene[a]	−69.291	1194.7	11.240	
Dimethylbenzene mixture[a]	−11.758	−1499.4	2.7243	
Ethanol[a]	−112.31	−1481.7	19.833	
1-Butanol[a]	−87.689	−2104.5	15.999	
Propanone[a]	−55.641	19.068	9.488	
Ethyl ethanoate[b]	−188.03	6434.2	28.986	4.4
2-Methylpropyl ethanoate[b]	−76.770	1509.3	12.373	2.5
Propanone[b]	−40.240	−587.3	7.152	7.4
Tetrahydrofuran[b]	2.900	−1600.7	0.252	6.9
Butanoic acid[b]	−150.15	4199.0	23.552	2.3
N,*N*-Dimethylformamide[b]	−52.982	341.7	8.873	4.4
1-Methyl-2-pyrrolidone[b]	−97.615	2991.6	15.198	4.9
Trichloromethane	48.913	−4126.1	−6.357	0.2
Tetrachloromethane	41.257	−4126.2	−5.049	0.2
1,1-Dichloroethane	47.077	−4126.1	−6.043	0.3
1,2-Dichloroethane	48.773	−4126.1	−6.333	0.3
Trichloroethene	44.512	−4126.1	−5.604	0.4
Tetrachloroethene	37.017	−4126.3	−4.325	0.2

[a] Numerical values of the coefficients were taken from Cui *et al.*[52]

[b] Numerical values of the coefficients were taken from Li *et al.*[53]

10.2. Naphthalene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Heptane; C_7H_{16}; [142-82-5]	[52]T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
290.25	0.9405	0.05948
294.30	0.9295	0.07054
297.85	0.9202	0.07982
301.37	0.9111	0.08893
303.04	0.9022	0.09778
305.30	0.8934	0.1066
307.53	0.8850	0.1150
309.63	0.8766	0.1234
311.20	0.8674	0.1326
312.60	0.8588	0.1412
314.13	0.8502	0.1498
315.15	0.8417	0.1583
316.63	0.8318	0.1682
317.65	0.8230	0.1770
321.33	0.7910	0.2090
324.25	0.7698	0.2302
326.98	0.7354	0.2646
329.45	0.6956	0.3044
330.26	0.6706	0.3294
331.50	0.6495	0.3505
333.75	0.6110	0.3890

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which the last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:

(1) Initial purity not given, Tianjin Kermel Chemical Reagent Purchase and Supply Station, China, was dissolved in acetone, filtered and the acetone evaporated. The sample was then recrystallized several times from methanol. The purity of the recrystallized sample was 99.8% as determined by UV spectrometry.

(2) 99.7%, Tianjin Kermel Chemical Reagent Company, Ltd, China, no information given regarding any further purification.

Estimated Error:

Temperature: ±0.2 K.

x_1: 5% (relative error).

TABLE 5. Parameters of the Buchowski λh equation for describing the solubility of naphthalene in various organic solvents[a]

Solvent	λ	h
Heptane	0.62352	9451.2
Methylbenzene	1.4722	2962.2
Dimethylbenzene mixture of isomers	1.6190	2906.0
Ethanol	0.62042	15 339.0
1-Butanol	1.8991	6048.3
Propanone	1.0642	4097.0

[a] Numerical values of the coefficients were taken from Cui *et al.*[52]

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Eicosane; $C_{20}H_{42}$; [112-95-8]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
309.79	1.0000	0.0000
309.42	0.8997	0.1003
308.89	0.7912	0.2088
307.30	0.6966	0.3034
317.40	0.5895	0.4105
323.20	0.4975	0.5025
330.90	0.4012	0.5988
337.37	0.3013	0.6987
343.46	0.2004	0.7996
348.36	0.0996	0.9004
352.55	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of naphthalene and eicosane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\text{K} = 307.6$ and eutectic mole fraction of naphthalene of $x_1 = 0.312$.

Auxiliary Information

Method/Apparatus/Procedure:

Differential scanning calorimeter.

The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:

(1) 99%, Prolabo, no purification details were given in the paper.

(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, purification details were not given in the paper.

Estimated Error:

Temperature: Authors state a global accuracy of ±1% regarding their measurements.

x_1: ± 0.0002 (estimated by compiler).

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Pentacosane; $C_{25}H_{52}$; [629-99-2]	[42]S. L. Hafsaoui and R. Mahmoud, J. Therm. Anal. Calorim. **88**, 565 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
324.10	1.000	0.000
323.72	0.899	0.101
321.48	0.800	0.200
318.13	0.702	0.298
317.38	0.599	0.401
324.23	0.501	0.499
330.20	0.401	0.599
336.70	0.302	0.698
344.48	0.199	0.801
348.14	0.102	0.898
353.42	0.000	1.000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Differential scanning calorimeter.

Mixtures of naphthalene and pentacosane were prepared by mass. The resulting mixtures were heated slowly with agitation until the entire sample melted. After melting the sample was immersed in liquid nitrogen to solidify the mixture completely. A small amount of solid was removed and sealed in a pan, the capsule was crimped, and placed in the calorimetric block of the differential scanning calorimeter for analysis.

Source and Purity of Chemicals:

(1) 99%, Fluka Chemical Company, was used as received.

(2) 99%, Fluka Chemical Company, was used as received.

Estimated Error:

Temperature: ±0.7 K.

x_1: ±0.002 (estimated by compiler).

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Pentacosane; $C_{25}H_{52}$; [629-99-2]	[54]P. M. Ghogomu, R. Rakolosaona, M. Bouroukba, D. Petitjean, N. Hubert, and M. Dirand, Mol. Cryst. Liq. Cryst. **408**, 103 (2004).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
327.05	1.000	0.000
326.65	0.874	0.126
325.45	0.768	0.232
324.85	0.675	0.325
323.35	0.593	0.407
322.15	0.524	0.476
320.85	0.426	0.574
319.05	0.356	0.644
321.45	0.308	0.698
336.75	0.268	0.732
345.15	0.144	0.856
348.65	0.085	0.915
350.65	0.036	0.964
354.05	0.000	1.000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Coupled simple thermal analysis–differential thermal analysis device constructed in the authors' laboratory.
Mixtures of naphthalene and pentacosane were prepared by mass, melted and mixed carefully, and then quenched in a crystallizing dish maintained at very low temperature. The solidified mixtures were ground to a fine powder and stored at ambient room temperature. The solidus-liquidus equilibrium temperature was determined by calorimetric methods using a coupled simple thermal analysis–differential thermal analysis device constructed in the authors' laboratory.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 98%, Fluka Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Octacosane; $C_{28}H_{58}$; [630-02-4]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
333.91	1.0000	0.0000
333.65	0.8970	0.1030
333.38	0.7990	0.2010
331.79	0.6997	0.3003
330.63	0.6003	0.3997
329.57	0.4976	0.5024
336.47	0.3505	0.6495
338.32	0.3004	0.6996
341.17	0.2505	0.7495
344.59	0.1993	0.8007
348.73	0.1000	0.9000
352.55	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of naphthalene and octacosane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 329.2$ and eutectic mole fraction of naphthalene of $x_1 = 0.524$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) 99%, Prolabo, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ±0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[59]A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.692	0.8871	0.1129

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 274 nm.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99.5%, Merck Chemical Company, Germany. No purification details were provided in the paper.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2% (relative error).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) *cis*-Decahydronaphthalene; $C_{10}H_{18}$; [493-01-6]

Original Measurements:
[55]T. Tsuji, K. Sue, T. Hiaki, and N. Itoh, Fluid Phase Equilib. **257**, 183 (2007).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
353.14	0.0000	1.0000
347.35	0.1073	0.8927
342.01	0.2024	0.7976
336.54	0.2985	0.7015
330.14	0.4178	0.5822
325.40	0.4971	0.5029
321.47	0.5488	0.4512
308.48	0.7041	0.2959
302.29	0.7631	0.2369
295.66	0.8045	0.1955
272.67	0.9087	0.0913
244.47	0.9642	0.0358
227.99	0.9800	0.0200
226.69	0.9895	0.0105
228.07	1.0000	0.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Pyrex glass sample cell, resistance thermometer, view type Dewar flask and a magnetic stirrer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the sample. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) 99.0%, Wako Pure Chemical Industries Ltd., Osaka, Japan, used as received.
(2) 97.0%, Wako Pure Chemical Industries Ltd. Gas chromatographic analysis showed the purity to be 97.8%. Sample was further purified by distillation by a rotary evaporator.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: <2% (relative error, estimated by compiler).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) *trans*-Decahydronaphthalene; $C_{10}H_{18}$; [493-02-7]

Original Measurements:
[55]T. Tsuji, K. Sue, T. Hiaki, and N. Itoh, Fluid Phase Equilib. **257**, 183 (2007).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
353.14	0.0000	1.0000
349.21	0.0687	0.9313
341.67	0.2164	0.7836
335.97	0.3245	0.6755
328.04	0.4634	0.5366
320.76	0.5739	0.4261
313.52	0.6539	0.3461
308.20	0.7117	0.2883
290.96	0.8272	0.1728
269.03	0.9244	0.0756
264.10	0.9384	0.0616
251.96	0.9610	0.0390
242.00	0.9798	0.0202
241.98	0.9864	0.0136
242.31	0.9899	0.0101
242.71	1.0000	0.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Pyrex glass sample cell, resistance thermometer, view type Dewar flask, and a magnetic stirrer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the sample. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) 99.0%, Wako Pure Chemical Industries Ltd., Osaka, Japan, used as received.
(2) 97.0%, Wako Pure Chemical Industries Ltd. Gas chromatographic analysis showed the purity to be 99.9%, and the chemical was used as received.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: <2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
327.75	0.4472	0.5528
332.05	0.3975	0.6025
335.55	0.3486	0.6514
338.55	0.2971	0.7029
341.05	0.2447	0.7553
344.05	0.1984	0.8016
346.35	0.1487	0.8513
348.65	0.0983	0.9017
350.55	0.0492	0.9508

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of naphthalene and squalane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 233.6$ and eutectic mole fraction of naphthalene of $x_1 = 0.04$.

Auxiliary Information

Method/Apparatus/Procedure:
Simple thermal analysis device constructed in the authors' laboratory, and a high precision platinum-resistance thermometer.
Phase diagram was determined using a simple thermal device. A sample of known composition was placed in a thermostatted glass tube, melted, and then slowly cooled at a rate of about 1 K/min. The temperature of the sample was measured with a high precision platinum-resistance thermometer. The crystallization temperature was obtained from a plot of the cooling curve versus time. Each measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Prolaboo, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

10.3. Naphthalene solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methylbenzene; C_7H_8; [108-88-3]	[52]T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
291.35	0.7605	0.2395
301.45	0.6897	0.3103
304.54	0.6604	0.3396
308.53	0.6261	0.3739
311.93	0.5945	0.4055
315.25	0.5613	0.4387
318.55	0.5283	0.4717
322.23	0.4973	0.5027
324.37	0.4629	0.5371
327.55	0.4111	0.5889
331.35	0.3626	0.6374
334.65	0.3227	0.6773

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) Initial purity not given, Tianjin Kermel Chemical Reagent Purchase and Supply Station, China, was dissolved in acetone, filtered and the acetone evaporated. The sample was then recrystallized several times from methanol. The purity of the recrystallized sample was 99.8% as determined by UV spectrometry.
(2) 99.5%, Tianjin Kermel Chemical Reagent Company, Ltd, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.16 K.
x_1: 2% (relative error).

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Dimethylbenzene (mixture of isomers); C_8H_{10} 13.3% 1,2-Dimethylbenzene; [95-47-6] 66.4% 1,3-Dimethylbenzene; [108-38-3] 20.3% 1,4-Dimethylbenzene; [106-42-3]	[52]T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
299.42	0.7082	0.2918
302.70	0.6821	0.3179
306.14	0.6566	0.3434
309.84	0.6285	0.3715
311.96	0.6019	0.3981
315.52	0.5605	0.4395
319.25	0.5209	0.4791
322.13	0.4917	0.5083
325.05	0.4554	0.5446
328.66	0.4198	0.5802
330.46	0.3914	0.6086
333.53	0.3533	0.6467
335.56	0.3150	0.6850
337.97	0.2804	0.7196

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:

(1) Initial purity not given, Tianjin Kermel Chemical Reagent Purchase and Supply Station, China, was dissolved in acetone, filtered and the acetone evaporated. The sample was then recrystallized several times from methanol. The purity of the recrystallized sample was 99.8% as determined by UV spectrometry.

(2) Mixture of isomers, Tianjin Kermel Chemical Reagent Company, Ltd, China, no information given regarding any further purification.

Estimated Error:

Temperature: ±0.1 K.
x_1: 1% (relative error).

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Biphenyl; $C_{12}H_{10}$; [92-52-4]	[39]A. C. Mengarelli, S. B. Bottini, and E. A. Brignole, J. Chem. Eng. Data **40**, 746 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_1[a]	x_2[b]
351.88	1.00	0.00
347.49	0.92	0.08
342.42	0.83	0.17
336.26	0.74	0.26
329.50	0.64	0.36
321.50	0.55	0.45
317.69	0.50	0.50
312.20	0.44	0.56
316.15	0.39	0.61
320.99	0.34	0.66
328.76	0.23	0.77
335.20	0.12	0.88
341.62	0.00	1.00

[a] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).
[b] x_2: mole fraction of component 2 in the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostatted liquid bath, platinum resistance thermometer, and a coiled wire driven by a small electrical motor to provide stirring.

A liquid mixture of known composition was prepared by mass and placed in a glass tube. The solution was slowly cooled until a solid phase appeared. The temperature of the solution was recorded continuously with a platinum resistance thermometer. A break point in the temperature versus time curve indicated formation of a solid phase. The temperature at break point was taken to be the solid-liquid equilibrium temperature, and the composition of the solution gives the solubility of the crystalline solute in the liquid solvent.

Source and Purity of Chemicals:

(1) Chemical purity and source not given in the paper.
(2) Chemical purity and source not given in the paper.

Estimated Error:

Temperature: ±0.5 K.
x_1: ± 0.01 (estimated by compiler).

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Phenanthrene; $C_{14}H_{10}$; [85-01-8]	[56]B. L. Sharma, R. Kant, R. Sharma, and S. Tandon, Mater. Chem. Phys. **82**, 216 (2003).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
373.0	1.0	0.0
364.0	0.9	0.1
356.0	0.8	0.2
348.0	0.7	0.3
339.0	0.6	0.4
329.0	0.5	0.5
326.0	0.4	0.6
334.0	0.3	0.7
340.0	0.2	0.8
346.5	0.1	0.9
353.0	0.0	1.0

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
The only experimental details provided in the paper was a statement by the authors that the solidus-liquid equilibrium data were obtained by the thaw-point melting technique.

Source and Purity of Chemicals:
(1) Laboratory Reagent Grade, Riedel Chemicals, was purified by sublimation.
(2) Analytical Reagent Grade, Fluka Chemicals, was purified by repeated recrystallizations from ethyl ethanoate.

Estimated Error:
Temperature: ±0.5 K (estimated by compiler).
x_1: ± 0.05 (estimated by compiler).

10.4. Naphthalene solubility data in esters

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[53]Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.20	0.8256	0.1744
283.17	0.8090	0.1910
288.21	0.7826	0.2174
293.19	0.7670	0.2330
298.25	0.7236	0.2764
303.20	0.6861	0.3139
308.21	0.6429	0.3571
313.23	0.5940	0.4060
318.17	0.5349	0.4651
323.21	0.4743	0.5257

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the inner chamber of a double-jacketed glass vessel. The vessel was maintained at a constant temperature by circulating water from a water bath equipped with a thermoelectric controller. The solute and solvent mixture was stirred with a magnetic stirrer. 1–3 mg of solute were added at predetermined intervals until no more solid would dissolve. Disappearance of the added solute was observed visually and with laser monitoring.

Source and Purity of Chemicals:
(1) 99%, Tianjin Kermel Chemical Reagent, China, was used as received.
(2) Research Grade, Shanghai Chemical Reagent, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2-Methylpropyl ethanoate; $C_6H_{12}O_2$; [110-19-0]	[53]Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.18	0.8169	0.1831
283.20	0.4953	0.2047
288.22	0.4681	0.2319
293.23	0.7407	0.2593
298.19	0.7011	0.2989
303.23	0.6655	0.3345
308.45	0.6135	0.3865
313.20	0.5673	0.4327
318.17	0.5166	0.4834
323.21	0.4607	0.5393

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the inner chamber of a double-jacketed glass vessel. The vessel was maintained at a constant temperature by circulating water from a water bath equipped with a thermoelectric controller. The solute and solvent mixture was stirred with a magnetic stirrer. 1–3 mg of solute were added at predetermined intervals until no more solid would dissolve. Disappearance of the added solute was observed visually and with laser monitoring.

Source and Purity of Chemicals:
(1) 99%, Tianjin Kermel Chemical Reagent, China, was used as received.
(2) Research Grade, Shanghai Chemical Reagent, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

10.5. Naphthalene solubility data in ethers

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[53]Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.60	0.7588	0.2412
284.35	0.7274	0.2726
288.25	0.7082	0.2918
293.25	0.6758	0.3242
298.00	0.6484	0.3516
303.20	0.6151	0.3849
308.19	0.5716	0.4284
313.25	0.5315	0.4685
318.35	0.4898	0.5102
323.20	0.4343	0.5657
328.21	0.4001	0.5999
333.22	0.3708	0.6292

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the inner chamber of a double-jacketed glass vessel. The vessel was maintained at a constant temperature by circulating water from a water bath equipped with a thermoelectric controller. The solute and solvent mixture was stirred with a magnetic stirrer. 1–3 mg of solute were added at predetermined intervals until no more solid would dissolve. Disappearance of the added solute was observed visually and with laser monitoring.

Source and Purity of Chemicals:
(1) 99%, Tianjin Kermel Chemical Reagent, China, was used as received.
(2) Research Grade, Shanghai Chemical Reagent, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methyl nonafluorobutyl ether; $C_5H_3F_9O$; [163702-07-6]	[60]A. F. Lagalante, A. Abdulagatov, and T. J. Bruno, J. Chem. Eng. Data **47**, 47 (2002).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
259.7	0.9982	0.00179
268.2	0.9974	0.00264
283.2	0.9932	0.00678
298.2	0.9893	0.0107
313.3	0.9867	0.0133
328.2	0.9680	0.0320

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
UV/visible spectrophotometer.
Solubilities were determined by supersaturating the solvent with naphthalene and measuring the amount of dissolved solute using a spectroscopic method. Aliquots of the saturated solution were pipette into a volumetric flask, and diluted with acetonitrile. If necessary, the sample was further diluted to bring the measured absorbance to within the linear range of the absorbance versus calibration curve obtained from absorbance measurements on solutions of known naphthalene concentration. Absorbance measurements recorded at 275 nm.

Source and Purity of Chemicals:
(1) Purity and Chemical Source were not given, was used as received.
(2) 99%, Name of commercial supplier was not given, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethyl nonafluorobutyl ether; $C_6H_5F_9O$; [163702-05-4]	[60]A. F. Lagalante, A. Abdulagatov, and T. J. Bruno, J. Chem. Eng. Data **47**, 47 (2002).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
259.7	0.9963	0.00374
268.2	0.9950	0.00500
283.2	0.9924	0.00763
298.2	0.9863	0.0137
313.3	0.9784	0.0216
328.2	0.7930	0.207
343.2	0.7390	0.261

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
UV/visible spectrophotometer.
Solubilities were determined by supersaturating the solvent with naphthalene and measuring the amount of dissolved solute using a spectroscopic method. Aliquots of the saturated solution were pipette into a volumetric flask, and diluted with acetonitrile. If necessary, the sample was further diluted to bring the measured absorbance to within the linear range of the absorbance versus calibration curve obtained from absorbance measurements on solutions of known naphthalene concentration. Absorbance measurements recorded at 275 nm.

Source and Purity of Chemicals:
(1) Purity and Chemical Source were not given, was used as received.
(2) 99%, Name of commercial supplier was not given, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

10.6. Naphthalene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.85	0.7501	0.2499
290.15	0.7415	0.2585
293.05	0.7214	0.2786
296.55	0.6956	0.3044
300.65	0.6633	0.3367
305.55	0.6215	0.3785
310.05	0.5799	0.4201
312.55	0.5554	0.4446
315.65	0.5237	0.4763
318.25	0.4959	0.5041
320.05	0.4759	0.5241
322.95	0.4426	0.5574

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute-solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, Polish Chemical Reagents, Gliwice, Poland, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.45	0.8070	0.1930
291.35	0.7892	0.2108
295.35	0.7623	0.2377
297.05	0.7498	0.2502
298.65	0.7375	0.2625
305.15	0.6848	0.3152
311.05	0.6301	0.3699
313.55	0.6048	0.3952
317.95	0.5566	0.4434
318.75	0.5480	0.4520
320.15	0.5319	0.4681
321.85	0.5107	0.4893

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute-solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, Polish Chemical Reagents, Gliwice, Poland, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) Purity not given, Polish Chemical Reagents, Gliwice, Poland, was dried over anhydrous sodium sulfate and then fractionally distilled.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) 1,1-Dichloroethane; $C_2H_4Cl_2$; [75-34-3]

Original Measurements:
[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.35	0.7663	0.2337
289.85	0.7566	0.2434
296.35	0.7105	0.2895
300.65	0.6773	0.3227
305.95	0.6313	0.3687
313.45	0.5601	0.4399
318.25	0.5086	0.4914
323.75	0.4457	0.5543

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute-solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, Polish Chemical Reagents, Gliwice, Poland, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) Purity not given, Polish Chemical Reagents, Glowice, Poland, was dried over anhydrous sodium sulfate and then fractionally distilled.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:
[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.35	0.7534	0.2466
291.65	0.7312	0.2688
294.15	0.7134	0.2866
296.55	0.6956	0.3044
298.55	0.6801	0.3199
302.55	0.6475	0.3525
306.05	0.6170	0.3830
308.55	0.5941	0.4059
310.05	0.5799	0.4201
313.05	0.5504	0.4496
315.05	0.5299	0.4701
316.85	0.5110	0.4890
318.55	0.4926	0.5074
320.05	0.4759	0.5241
321.85	0.4555	0.5445

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, electric glass furnace, heater, mercury thermometer.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute-solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of stereoscopic microscope.

Source and Purity of Chemicals:
(1) Analytically pure, Polish Chemical Reagents, Gliwice, Poland, recrystallized twice from distilled benzene and then from anhydrous ethanol.
(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.3 K.
x_1: < 1% (relative error).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Trichloroethene; C_2HCl_3; [79-01-6]

Original Measurements:
[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.35	0.7839	0.2161
290.85	0.7679	0.2321
298.55	0.7126	0.2874
300.85	0.6944	0.3056
303.35	0.6735	0.3265
310.15	0.6115	0.3885
315.85	0.5531	0.4469
318.45	0.5244	0.4756
321.75	0.4861	0.5139
323.25	0.4679	0.5321

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, electric glass furnace, heater, mercury thermometer.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute-solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of stereoscopic microscope.

Source and Purity of Chemicals:

(1) Analytically pure, Polish Chemical Reagents, Gliwice, Poland, recrystallized twice from distilled benzene and then from anhydrous ethanol.

(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:

Temperature: ±0.3 K.

x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Tetrachloroethene; C_2Cl_4; [127-18-4]	[13]I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.45	0.8324	0.1676
290.65	0.8196	0.1804
292.65	0.8071	0.1929
294.45	0.7957	0.2043
294.85	0.7932	0.2068
296.25	0.7840	0.2160
297.95	0.7712	0.2288
302.65	0.7350	0.2650
306.15	0.7055	0.2945
309.65	0.6734	0.3266
312.45	0.6458	0.3542
318.35	0.5819	0.4181
323.95	0.5139	0.4861

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, electric glass furnace, heater, mercury thermometer.

Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a Pyrex test tube and sealed by a flexible rubber cap mounted on a calibrated mercury thermometer. The solute-solvent were heated using an electrical glass furnace equipped with a platinum resistor placed near the heater. Samples were agitated and the temperature at which the solid solute disappeared was observed against a dark screen by means of stereoscopic microscope.

Source and Purity of Chemicals:

(1) Analytically pure, Polish Chemical Reagents, Gliwice, Poland, recrystallized twice from distilled benzene and then from anhydrous ethanol.

(2) 99.5+%, purchased from either Fluka or Aldrich Chemical Company, was used as received.

Estimated Error:

Temperature: ±0.3 K.

x_1: < 1% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	[57]D. Wei and K. Jin, J. Chem. Thermodyn. **41**, 145 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
255.85	1.0000	0.0000
244.25	0.9711	0.0289
240.65	0.9251	0.0749
252.15	0.8579	0.1421
270.75	0.7910	0.2090
278.25	0.7568	0.2432
285.35	0.7199	0.2801
289.25	0.7018	0.2982
295.65	0.6585	0.3415
304.95	0.6036	0.3964
309.15	0.5700	0.4300
313.55	0.5331	0.4669
319.45	0.4710	0.5290
323.35	0.4388	0.5612
329.45	0.3770	0.6230
330.65	0.3510	0.6490
336.65	0.2787	0.7213
339.25	0.2308	0.7692
344.45	0.1529	0.8471
347.65	0.1098	0.8902
349.15	0.0779	0.9221
353.25	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the system is of an incongruent eutectic type. The eutectic point occurs at $T/\text{K} = 232.55$ and $x_1 = 0.130$, and the peritectic point occurs at $T/\text{K} = 250.15$ and $x_1 = 0.077$. The composition of the incongruent compound is a molar ratio of 1:1 between naphthalene and 1,2-dichlorobenzene.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
Phase diagram was determined using a differential scanning calorimeter. Samples of naphthalene and dichlorobenzene were heated very slowly inside a glass tube near the melting point of the major component. The fluid solution was then allowed to solidify with continuous stirring. A small quantity of the solid material was then sealed into a dsc sampling crucible for analysis. Measurements were performed at a constant fixed scanning rate of 1 K/min.

Source and Purity of Chemicals:
(1) 99.5+%, Analytical Research Grade, Tianjin Kewei Chemical Reagent Company, China, was used as received.
(2) 99.5+%, Analytical Research Grade, Tianjin Kewei Chemical Reagent Company, China, was used as received.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]	[57]D. Wei and K. Jin, J. Chem. Thermodyn. **41**, 145 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
248.25	1.0000	0.0000
261.15	0.8886	0.1114
272.35	0.8420	0.1580
283.45	0.7822	0.2178
293.05	0.7189	0.2811
299.25	0.6750	0.3250
304.15	0.6329	0.3671
311.65	0.5640	0.4360
317.55	0.5038	0.4962
321.85	0.4542	0.5458
324.15	0.4299	0.5701
326.55	0.4030	0.5970
331.05	0.3420	0.6580
334.45	0.2949	0.7051
336.35	0.2679	0.7321
338.15	0.2458	0.7542
340.95	0.2038	0.7962
343.65	0.1681	0.8319
346.15	0.1252	0.8748
347.95	0.0918	0.9082
349.15	0.0711	0.9289
350.95	0.0429	0.9571
353.25	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the system is of an incongruent eutectic type. The eutectic point occurs at $T/\mathrm{K} = 244.85$ and $x_1 = 0.058$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
Phase diagram was determined using a differential scanning calorimeter. Samples of naphthalene and dichlorobenzene were heated very slowly inside a glass tube near the melting point of the major component. The fluid solution was then allowed to solidify with continuous stirring. A small quantity of the solid material was then sealed into a dsc sampling crucible for analysis. Measurements were performed at a constant fixed scanning rate of 1 K/min.

Source and Purity of Chemicals:
(1) 99.5+%, Analytical Research Grade, Tianjin Kewei Chemical Reagent Company, China, was used as received.
(2) 99.5+%, Analytical Research Grade, Tianjin Kewei Chemical Reagent Company, China, was used as received.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]	[57]D. Wei and K. Jin, J. Chem. Thermodyn. **41**, 145 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
326.15	1.0000	0.0000
321.95	0.9263	0.0737
317.05	0.8500	0.1500
314.15	0.8078	0.1922
311.65	0.7630	0.2370
310.65	0.7437	0.2563
307.15	0.6938	0.3062
305.15	0.6562	0.3438
306.25	0.5772	0.4228
312.35	0.5169	0.4831
320.15	0.4410	0.5590
326.65	0.3740	0.6260
331.35	0.3157	0.6843
335.05	0.2689	0.7311
339.65	0.2042	0.7958
343.55	0.1568	0.8432
347.95	0.0791	0.9209
350.75	0.0470	0.9530
353.25	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors report that the system is of a simple eutectic type. The eutectic point occurs at $T/\mathrm{K} = 302.85$ and $x_1 = 0.390$.

Auxiliary Information

Method/Apparatus/Procedure:

Differential scanning calorimeter.

The phase diagram was determined using a differential scanning calorimeter. Samples of naphthalene and dichlorobenzene were heated very slowly inside a glass tube near the melting point of the major component. The fluid solution was then allowed to solidify with continuous stirring. A small quantity of the solid material was then sealed into a dsc sampling crucible for analysis. Measurements were performed at a constant fixed scanning rate of 1 K/min.

Source and Purity of Chemicals:

(1) 99.5+%, Analytical Research Grade, Tianjin Kewei Chemical Reagent Company, China, was used as received.

(2) 99.5+%, Analytical Research Grade, Tianjin Kewei Chemical Reagent Company, China, was used as received.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±0.002 (estimated by compiler).

10.7. Naphthalene solubility data in alcohols

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Methanol; CH_4O; 67-56-1]	[59]A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.540	0.9771	0.0229

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:

Incubator, shaker, and an ultraviolet/visible spectrophotometer.

Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 274 nm.

Source and Purity of Chemicals:

(1) 99%, Fluka Chemical Company, was used as received.

(2) 99.5%, Merck Chemical Company, Germany. No purification details were provided in the paper.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5]	[59]A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.558	0.9664	0.0336

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:

Incubator, shaker, and an ultraviolet/visible spectrophotometer.

Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 274 nm.

Source and Purity of Chemicals:

(1) 99%, Fluka Chemical Company, was used as received.

(2) 99.5%, Merck Chemical Company, Germany. No purification details were provided in the paper.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5]	[52]T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
304.26	0.9536	0.04640
307.44	0.9469	0.05311
309.53	0.9434	0.05656
311.93	0.9386	0.06141
314.52	0.3642	0.06584
315.93	0.9297	0.07025
318.07	0.9240	0.07601
319.80	0.9184	0.08161
321.46	0.9124	0.08761
323.45	0.8965	0.1035
325.68	0.8838	0.1162
327.32	0.8715	0.1285
329.34	0.8605	0.1395
330.43	0.8461	0.1539
332.00	0.8258	0.1742
333.90	0.7964	0.2036
335.90	0.7618	0.2382
337.76	0.7065	0.2935
339.76	0.6185	0.3815

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which the last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) Initial purity not given, Tianjin Kermel Chemical Reagent Purchase and Supply Station, China, was dissolved in acetone, filtered and the acetone evaporated. The sample was then recrystallized several times from methanol. The purity of the recrystallized sample was 99.8% as determined by UV spectrometry.
(2) 99.7%, Tianjin Kermel Chemical Reagent Company, Ltd, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: 3% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	[59]A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.601	0.9539	0.0461

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotometric analysis at 274 nm.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99.5%, Merck Chemical Company, Germany. No purification details were provided in the paper.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2-Propanol: C_3H_8O; [67-63-0]	[59]A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.571	0.9549	0.0451

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 274 nm.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99.5%, Merck Chemical Company, Germany. No purification details were provided in the paper.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[59]A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.705	0.9339	0.0661

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 274 nm.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99.5%, Merck Chemical Company, Germany. No purification details were provided in the paper.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[52]T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
313.77	0.8873	0.1127
315.17	0.8805	0.1195
317.98	0.8612	0.1388
320.74	0.8410	0.1590
323.67	0.8172	0.1828
325.60	0.7954	0.2046
327.76	0.7721	0.2279
329.03	0.7476	0.2524
331.80	0.7063	0.2937
333.65	0.6674	0.3326
335.10	0.6251	0.3749
337.00	0.5637	0.4363
338.15	0.5234	0.4766
339.63	0.4735	0.5265
340.65	0.4326	0.5674
342.04	0.3803	0.6197
342.80	0.3395	0.6605

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which the last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) Initial purity not given, Tianjin Kermel Chemical Reagent Purchase and Supply Station, China, was dissolved in acetone, filtered and the acetone evaporated. The sample was then recrystallized several times from methanol. The purity of the recrystallized sample was 99.8% as determined by UV spectrometry.
(2) 99.0%, Tianjin Kermel Chemical Reagent Company, Ltd, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.15 K.
x_1: 2% (relative error).

10.8. Naphthalene solubility data in ketones

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Propanone; C_3H_6O; [67-64-1]	[53]Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8763	0.1237
283.15	0.8567	0.1433
288.05	0.8293	0.1707
293.25	0.8059	0.1941
298.15	0.7740	0.2260
303.00	0.7319	0.2681
308.10	0.6927	0.3073
313.05	0.6394	0.3606
318.15	0.5825	0.4175
323.05	0.5229	0.4771

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the inner chamber of a double-jacketed glass vessel. The vessel was maintained at a constant temperature by circulating water from a water bath equipped with a thermoelectric controller. The solute and solvent mixture was stirred with a magnetic stirrer. 1–3 mg of solute were added at predetermined intervals until no more solid would dissolve. Disappearance of the added solute was observed visually and with laser monitoring.

Source and Purity of Chemicals:
(1) 99%, Tianjin Kermel Chemical Reagent, China, was used as received.
(2) Research Grade, Shanghai Chemical Reagent, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Propanone; C_3H_6O; [67-64-1]	[52]T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.17	0.7894	0.2106
298.11	0.7815	0.2185
300.23	0.7671	0.2329
301.55	0.7540	0.2460
303.47	0.7411	0.2589
305.14	0.7276	0.2724
306.63	0.7154	0.2846
307.76	0.7028	0.2972
309.37	0.6899	0.3101
311.03	0.6770	0.3230
312.03	0.6654	0.3346
312.97	0.6532	0.3468
314.37	0.6392	0.3608
315.74	0.6238	0.3762
317.26	0.6058	0.3942
319.06	0.5846	0.4154
320.87	0.5603	0.4397
322.70	0.5414	0.4586

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in a dissolving flask. The solid in the solution dissolved as the temperature was increased. The temperature at which the last amount of solid dissolved was recorded as the solid-liquid equilibrium temperature. The disappearance of the solid solute was determined by laser monitoring.

Source and Purity of Chemicals:
(1) Initial purity not given, Tianjin Kermel Chemical Reagent Purchase and Supply Station, China, was dissolved in acetone, filtered and the acetone evaporated. The sample was then recrystallized several times from methanol. The purity of the recrystallized sample was 99.8% as determined by UV spectrometry.
(2) 99.5%, Tianjin Kermel Chemical Reagent Company, Ltd, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: 0.7% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1,2-Diphenyl-1,2-ethanedione; $C_{14}H_{10}O_2$; [134-81-6]	[58]U. S. Rai and R. N. Rai, Asian J. Chem. **10**, 421 (1998).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

The binary phase diagram was graphically depicted in the paper. The phase diagram showed formation of a simple eutectic at T/K = 372 and a mole fraction composition of naphthalene of $x_1 = 0.592$.

Auxiliary Information

Method/Apparatus/Procedure:
Melting-point apparatus equipped with a precision thermometer.
The phase diagram was determined by the thaw-melt method. Binary mixtures of the two components were prepared by mass, placed in a test tube, and homogenized by repeated melting and thawing. The melting point and thawing temperature for the phase diagram was determined using a melting point apparatus equipped with a precision thermometer.

Source and Purity of Chemicals:
(1) Purity not given, Fluka Chemicals, purified by sublimation followed by recrystallization from cyclohexane.
(2) Purity not given, CDH, China, was purified by repeated recrystallization from ethyl ethanoate.

Estimated Error:
Temperature: ±0.5 K.
x_1: 0.005 (estimated by compiler).

10.9. Naphthalene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) *N,N*-Dimethylformamide; C_3H_7NO; [111-84-2]	[53]Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.05	0.8385	0.1615
283.05	0.8148	0.1852
288.15	0.7850	0.2150
292.75	0.7556	0.2444
298.05	0.7186	0.2814
303.25	0.6929	0.3071
307.95	0.6461	0.3539
313.15	0.5941	0.4059
318.15	0.5351	0.4649

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the inner chamber of a double-jacketed glass vessel. The vessel was maintained at a constant temperature by circulating water from a water bath equipped with a thermoelectric controller. The solute and solvent mixture was stirred with a magnetic stirrer. 1–3 mg of solute were added at predetermined intervals until no more solid would dissolve. Disappearance of the added solute was observed visually and with laser monitoring.

Source and Purity of Chemicals:
(1) 99%, Tianjin Kermel Chemical Reagent, China, was used as received.
(2) Research Grade, Shanghai Chemical Reagent, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[53]Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.18	0.7315	0.2685
283.25	0.7107	0.2893
288.17	0.6927	0.3073
293.20	0.6642	0.3358
298.16	0.6215	0.3785
303.21	0.5899	0.4101
308.17	0.5617	0.4383
313.16	0.5136	0.4864
318.21	0.4654	0.5346
323.27	0.4233	0.5767

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Double-jacketed glass vessel, laser generator, water bath, photoelectric transformer, and digital display.
Solubilities were determined by a synthetic-dynamic method. Known masses of solute and solvent were placed in the inner chamber of a double-jacketed glass vessel. The vessel was maintained at a constant temperature by circulating water from a water bath equipped with a thermoelectric controller. The solute and solvent mixture was stirred with a magnetic stirrer. 1–3 mg of solute were added at predetermined intervals until no more solid would dissolve. Disappearance of the added solute was observed visually and with laser monitoring.

Source and Purity of Chemicals:
(1) 99%, Tianjin Kermel Chemical Reagent, China, was used as received.
(2) Research Grade, Shanghai Chemical Reagent, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

---

11. Solubility of Phenanthrene in Organic Solvents

11.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained experimental solubility data for phenanthrene dissolved in four linear alkanes (hexane, heptane, octane, and octadecane) and two cycloalkanes (cyclohexane and decahydronaphthalene), in three aromatic hydrocarbons (benzene, methylbenzene, and 1,2,3,4-tetrahydronaphthalene), in three halogenated alkanes (tetrachloromethane, 1-hydroperfluoroheptane, and 1,8-dihydroperfluorooctane), in two alkanols (methanol and 1-octanol), and in five miscellaneous organic solvents (pyridine, thiophene, perfluorotributylamine, nitrobenzene, and carbon disulfide). The volume also included phase diagram information for binary phenanthrene + biphenyl, phenanthrene + fluoranthene, phenanthrene + acenaphthene, phenanthrene + 1,4-dibromobenzene, phenanthrene + 1,4-dibromobenzene, phenanthrene + octafluoronaphthalene, phenanthrene + 1,2-dinitrobenzene, phenanthrene + 1,3-dinitrobenzene, phenanthrene + 1,4-dinitrobenzene, phenanthrene + 1,3,5-trinitrobenzene, phenanthrene + 1,2,3,5-tetranitrobenzene, phenanthrene + 2,4-dinitromethylbenzene, phenanthrene + 2,6-dinitromethylbenzene, phenanthrene + 3,4-dinitromethylbenzene, phenanthrene + 2,4,6-trinitromethylbenzene, phenanthrene + 2,4-dinitrophenol, phenanthrene + 1-chloro-4-nitrobenzene, phenanthrene + dibenzothiophene, phenanthrene + thianthrene, phenanthrene + benzoic acid, phenanthrene + *trans*-cinnamic acid, phenanthrene + 2-hydroxybenzoic acid, phenanthrene + 3-hydroxybenzoic acid, and phenanthrene + 6-methyl-2,3,4-trinitrophenol mixtures. Solubility data contained in Vol. 59 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for phenanthrene.

After Vol. 59 appeared in print, there have been several experimental solubility studies involving phenanthrene in organic solvents. Acree and co-workers[17,62] measured the solubility of anthracene in eight linear alkanes (hexane, heptane, octane, nonane, decane, undecane, dodecane, and hexadecane), four cycloalkanes (cyclohexane, methylcyclohexane, cyclooctane, and *tert*-butylcyclohexane) and one branched alkane (2,2,4-trimethylpentane), in two alkyl alkanoates (ethyl ethanoate and butyl ethanoate), in one dialkyl ether (1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in one chloroalkane (tetrachloromethane), in 14 primary alkanols (methanol, ethanol, 1-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 1-heptanol, 1-octanol, 2-ethyl-1-hexanol, 1,2-ethanediol, and 2,2,2-trifluoroethanol), in five secondary alkanols (2-propanol, 2-butanol, 2-pentanol, 4-methyl-2-pentanol, and cyclopentanol) and one tertiary alkanol (2-methyl-2-butanol), in two alkanones (butanone, cyclohexanone), and in three miscellaneous organic solvents (ethanenitrile, propanenitrile, and butanenitrile). For the majority of the solvents studied by Acree and coworkers there is only the single experimental value, and it is not possible to perform a critical evaluation on most of the published data.

There do exist independent solubility measurements for phenanthrene dissolved in 2,2,4-trimethylpentane and in several of the smaller alkanols. Shayanfar *et al.*[34] measured the solubility of phenanthrene in binary 2,2,4-trimethylpentane and ethanol mixtures at 298.2, 308.2, and 318.2 K. The authors measured mole fraction solubilities at 298.2 K in 2,2,4-trimethylpentane ($x_1 = 0.0246$) and ethanol ($x_1 = 0.0119$) were in reasonably good agreement with the earlier published values of $x_1 = 0.002486$ for 2,2,4-trimethylpentane and $x_1 = 0.001114$ for ethanol determined by Hernández *et al.*[61] Since only three temperatures were studied by Shayanfar *et al.*,[34] it is not feasible to use the three-parameter Apelblat equation to assess the internal consistency of the authors' experimental data since the equation would yield essentially a perfect fit. There is one additional independent experimental measurement for the solubility of phenanthrene in ethanol. Fakhree *et al.*[62,63] measured the solubilities of phenanthrene in binary and ternary mixtures of C_1–C_4 alcohols. The measured mole fraction solubilities compare favorably with the values determined by Acree and co-workers,[17,62] namely, $x_1 = 0.00549$ versus $x_1 = 0.00589$ for methanol, $x_1 = 0.0108$ versus $x_1 = 0.01114$ for ethanol, $x_1 = 0.0132$ versus $x_1 = 0.01355$ for 1-propanol, and $x_1 = 0.0178$ versus $x_1 = 0.01771$ for 1-butanol.

Lisicki and Jamróz[35] reported solid-liquid equilibria data for binary mixtures containing phenanthrene with *N*,*N*-dimethylacetamide, 1-methyl-2-pyrrolidone, and hexahydro-1-methyl-2*H*-azepin-2-one (also called *N*-methyl-ε-caprolactam). The phenanthrene + *N*,*N*-dimethylformamide and phenanthrene + 1-methyl-2-pyrrolidone systems both exhibited simple eutectic behavior. The published experimental liquidus curves for the latter three phenanthrene systems did not indicate any outlier data points.

The experimental solubility data for phenanthrene dissolved in the different organic solvents are given in Secs. 11.2–11.9.

11.2. Phenanthrene solubility data in saturated hydrocarbons (including cycloalkanes)

Components: (1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Hexane; C_6H_{14}; [110-54-3]	**Original Measurements:** [61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9681	0.03189

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Heptane; C_7H_{16}; [142-82-5]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9611	0.03888

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Octane; C_8H_{18}; [111-65-9]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9556	0.04443

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Nonane; C_9H_{20}; [111-84-2]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9522	0.04785

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9447	0.05531

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Undecane; $C_{11}H_{24}$; [1120-21-4]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9402	0.05980

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in undecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Dodecane; $C_{12}H_{26}$; [112-40-3]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9365	0.06348

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in dodecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9203	0.07972

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Octacosane; $C_{28}H_{58}$; [630-02-4]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
333.91	1.0000	0.0000
333.81	0.8969	0.1031
333.22	0.8004	0.1996
331.26	0.6915	0.3085
341.01	0.5001	0.4999
344.75	0.4485	0.5515
350.95	0.4004	0.5996
360.10	0.2801	0.7199
364.14	0.2000	0.8000
367.60	0.1002	0.8998
371.35	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of phenanthrene and octacosane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of T/K = 329.0 and eutectic mole fraction of phenanthrene of $x_1 = 0.420$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9635	0.03648

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9543	0.04572

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9400	0.06002

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9751	0.02486

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[34]A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
298.2	0.9754	0.0246
308.2	0.9622	0.0378
318.2	0.9516	0.0484

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 356 nm.

Source and Purity of Chemicals:
(1) 98%, Merck Chemicals, Germany, was recrystallized several times from propanone before use.
(2) 99+%, Merck Chemicals, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2.5% (relative uncertainty).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9488	0.05124

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
331.65	0.6984	0.3016
343.15	0.5953	0.4047
353.15	0.4803	0.5197
356.55	0.4463	0.5537
359.25	0.3967	0.6033
360.75	0.3501	0.6499
362.55	0.2939	0.7061
363.95	0.2497	0.7503
365.15	0.2021	0.7979
366.35	0.1540	0.8460
367.65	0.0988	0.9012
369.15	0.0507	0.9493

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of phenanthrene and squalane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 233.8$ and eutectic mole fraction of phenanthrene of $x_1 = 0.03$.

Auxiliary Information

Method/Apparatus/Procedure:
Simple thermal analysis device constructed in the authors' laboratory, and a high precision platinum-resistance thermometer.
Phase diagram was determined using a simple thermal device. A sample of known composition was placed in a thermostatted glass tube, melted and then slowly cooled at a rate of about 1 K/min. The temperature of the sample was measured with a high precision platinum-resistance thermometer. The crystallization temperature was obtained from a plot of the cooling curve versus time. Each measurement was repeated three times.

Source and Purity of Chemicals:
(1) 98+%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

11.3. Phenanthrene solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Methylbenzene; C_7H_8; [108-88-3]	[64]Y. Bakhbakhi, P. Charpentier, and S. Rohani, Can. J. Chem. Eng. **83**, 267 (2005).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a,b]	x_1[b,c]
298.15	0.8099	0.1901
303.15	0.7821	0.2179
308.15	0.7514	0.2486
313.15	0.7185	0.2815
318.15	0.6798	0.3202
323.15	0.6406	0.3594
328.15	0.5964	0.4036
333.15	0.5520	0.4480
338.15	0.5033	0.4967

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] Experimental values based on ATR-FTIR method.
[c] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Solubilities were reported in the paper as the grams of phenanthrene dissolved per 100 g of solvent. Mole fraction solubilities were calculated by the compiler.

Experimental Values

T/K	x_2[a,b]	x_1[b,c]
298.15	0.8029	0.1971
303.15	0.7953	0.2047
308.15	0.7627	0.2373
313.15	0.7293	0.2707
318.15	0.6846	0.3154
323.15	0.6499	0.3501
328.15	0.5988	0.4012
333.15	0.5587	0.4413
338.15	0.5033	0.4967

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] Experimental values based on gravimetric method.
[c] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Solubilities were reported in the paper as the grams of phenanthrene dissolved per 100 g of solvent. Mole fraction solubilities were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Three-neck glass vessel, attenuated total reflectance FTIR spectrophotometer; regular diamond immersion probe, temperature controller.
Solubilities were determined by a synthetic-undersaturation method. Known masses of solute and solvent were placed in a three-neck glass vessel. Once equilibrium is achieved a steady-stated ATR-FTIR reading is recorded. An additional known mass of phenanthrene is added to the solution. Once equilibrium is achieved, a new steady-state ATR-FTIR reading is recorded and compared to the previous reading. As long as there is no change in FTIR reading, the measurement is taken as the solubility of phenanthrene at the solution temperature. If the reading has changed, additional phenanthrene is added until a saturated solution is obtained. The authors checked the method by performing phenanthrene solubility measurements using a gravimetric method. The solubilities determined using the gravimetric and ATR-FTIR methods were in good agreement.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, USA, no further purification details were provided in the paper.
(2) Analytical Grade, Sigma-Aldrich Chemical Company, USA, no further purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: 2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Naphthalene; $C_{10}H_8$; [91-20-3]	[56] B. L. Sharma, R. Kant, R. Sharma, and S. Tandon, Mater. Chem. Phys. **82**, 216 (2003).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_1[a]	x_2[b]
373.0	1.0	0.0
364.0	0.9	0.1
356.0	0.8	0.2
348.0	0.7	0.3
339.0	0.6	0.4
329.0	0.5	0.5
326.0	0.4	0.6
334.0	0.3	0.7
340.0	0.2	0.8
346.5	0.1	0.9
353.0	0.0	1.0

[a] x_1: mole fraction of the component 1 in the saturated solution.
[b] x_2: mole fraction of component 2 in the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
The only experimental details provided in the paper was a statement by the authors that the solidus-liquid equilibrium data were obtained by the thaw-point melting technique.

Source and Purity of Chemicals:
(1) Analytical Reagent Grade, Fluka Chemicals, was purified by repeated recrystallizations from ethyl ethanoate.
(2) Laboratory Reagent Grade, Riedel Chemicals, was purified by sublimation.

Estimated Error:
Temperature: ±0.5 K (estimated by compiler).
x_1: ± 0.05 (estimated by compiler).

11.4. Phenanthrene solubility data in esters

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[61] C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.8501	0.1499

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8188	0.1812

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

11.5. Phenanthrene solubility data in ethers

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2); 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9055	0.09454

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.7116	0.2884

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.7835	0.2165

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

11.6. Phenanthrene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Tetrachloromethane; CCl_4; [56-23-5]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8738	0.1262

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

11.7. Phenanthrene solubility data in alcohols

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Methanol; CH_4O; [67-56-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9941	0.00589

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Methanol; CH_4O; [67-56-1]	[62]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.133	0.9945	0.00549

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 345 nm.

Source and Purity of Chemicals:
(1) 99%, Merck Chemical Company, Germany, was recrystallized several times from propanone.
(2) 99.5%, Merck Chemical Company. No purification details were provided in the paper. Water content was checked by Karl Fischer titration and found to be 0.04% by mass.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Ethanol; C_2H_6O; [64-17-5]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9889	0.01114

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Ethanol; C_2H_6O; [64-17-5]	[34]A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9881	0.0119
308.2	0.9841	0.0159
318.2	0.9810	0.0190

[a] x_2: mole fraction of the component 2 in the saturated solution.
[b] x_1: mole fraction of component 1 in the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 356 nm.

Source and Purity of Chemicals:
(1) 98%, Merck Chemicals, Germany, was recrystallized several times from propanone before use.
(2) 99+%, Absolute, Merck Chemicals, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±2.5% (relative uncertainty).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Ethanol; C_2H_6O; [64-17-5]	[62]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.182	0.9892	0.0108

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 345 nm.

Source and Purity of Chemicals:
(1) 99%, Merck Chemical Company, Germany, was recrystallized several times from propanone.
(2) 99.9%, Merck Chemical Company. No purification details were provided in the paper. Water content was checked by Karl Fischer titration and found to be 0.13% by mass.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Propanol; C_3H_8O; [71-23-8]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9865	0.01355

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Propanol; C_3H_8O; [71-23-8]	[62]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.174	0.9868	0.0132

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 345 nm.

Source and Purity of Chemicals:
(1) 99%, Merck Chemical Company, Germany, was recrystallized several times from propanone.
(2) 99.5%, Merck Chemical Company. No purification details were provided in the paper. Water content was checked by Karl Fischer titration and found to be 0.07% by mass.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Propanol; C_3H_8O; [67-63-0]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9902	0.00977

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9823	0.01771

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[62]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.194	0.9822	0.0178

[a] c_1: molar solubility of the solute.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The mole fraction solubility of the solute was calculated by the compiler using the experimental density data given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 345 nm.

Source and Purity of Chemicals:
(1) 99%, Merck Chemical Company, Germany, was recrystallized several times from propanone.
(2) 99.5%, Merck Chemical Company. No purification details were provided in the paper. Water content was checked by Karl Fischer titration and found to be 0.40% by mass.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9882	0.01178

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9898	0.01020

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9751	0.02491

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9824	0.01764

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9839	0.01606

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]

Original Measurements:
[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9807	0.01926

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

Original Measurements:
[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9697	0.03028

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]

Original Measurements:
[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9820	0.01801

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9825	0.01754

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9606	0.03937

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9458	0.05418

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9712	0.02876

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9693	0.03070

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9989	0.001134

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9982	0.001826

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

11.8. Phenanthrene solubility data in ketones

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2-Butanone; C_4H_8O; [78-93-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.7910	0.2090

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.7284	0.2716

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

11.9. Phenanthrene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9673	0.03267

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Propanenitrile; C_3H_5N; [107-12-0]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8794	0.1206

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Butanenitrile; C_4H_7N; [109-74-0]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8376	0.1624

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 347 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
253.2	1.0000	0.0000
252.7	0.9900	0.0100
251.3	0.9712	0.0288
250.2	0.9497	0.0503
249.2	0.9395	0.0605
248.1	0.9249	0.0751
245.9	0.9006	0.0994
250.7	0.8797	0.1203
260.2	0.8508	0.1492
274.8	0.8009	0.1991
287.8	0.7509	0.2491
298.4	0.8968	0.3032
308.3	0.6385	0.3615
314.3	0.5997	0.4003
318.4	0.5713	0.4287
328.0	0.4974	0.5026
339.6	0.3915	0.6085
349.1	0.2942	0.7058
359.4	0.1812	0.8188
366.4	0.0959	0.9041
372.9	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 245.5$ and eutectic composition of $x_1 = 0.105$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature-controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Koch-Light Lab. Ltd., United Kingdom, was purified with concentrated sulfuric acid, followed by maleic anhydride, and then recrystallized to yield a sample of 99.86% purity (mass percent).
(2) Purest grade, Merck-Schuchardt, Federal Republic of Germany, was distilled under reduced pressure and dried over molecular sieves to produce a sample of 99.9% purity (mass percent).

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 1-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
248.5	1.0000	0.0000
248.1	0.9898	0.0102
246.5	0.9507	0.0493
245.3	0.9249	0.0751
243.8	0.8993	0.1007
246.7	0.8570	0.1430
262.9	0.8009	0.1991
275.0	0.7520	0.2480
278.3	0.7340	0.2660
280.4	0.7274	0.2726
282.8	0.7139	0.2861
288.4	0.6920	0.3080
293.4	0.6663	0.3337
305.4	0.5964	0.4036
319.4	0.4988	0.5012
330.0	0.4197	0.5803
335.1	0.3800	0.6200
340.7	0.3328	0.6672
356.8	0.2020	0.7980
365.3	0.0996	0.9004
372.9	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors reported that the binary system exhibits simple eutectic behavior, with a eutectic temperature of $T/\mathrm{K} = 242.4$ and eutectic composition of $x_1 = 0.162$.

Auxiliary Information

Method/Apparatus/Procedure:
Temperature controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Koch-Light Lab. Ltd., United Kingdom, was purified with concentrated sulfuric acid, followed by maleic anhydride, and then recrystallized to yield a sample of 99.86% purity (mass percent).
(2) Technical Grade, BASF, Federal Republic of Germany, was purified by treatment with a 2% solution of potassium permanganate, and then distilled under reduced pressure to collect the distillate having 99.8% purity (mass percent). The purified sample was dried over molecular sieves.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Hexahydro-1-methyl-2*H*-azepin-2-one (*N*-Methyl-ε-caprolactam); $C_7H_{13}NO$; [2556-73-2]	[35]Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
279.6	1.0000	0.0000
281.3	0.7225	0.2775
294.1	0.6749	0.3251
300.2	0.6363	0.3637
308.4	0.5992	0.4008
316.3	0.5479	0.4521
323.6	0.5044	0.4956
325.2	0.4988	0.5012
334.9	0.4207	0.5793
343.5	0.3464	0.6536
353.5	0.2480	0.7520
362.1	0.1497	0.8503
369.7	0.0486	0.9514
372.9	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Temperature controlled heating/cooling system and a shaking-mixing system. Synthetic mixtures of known compositions were weighed in small glass ampoules. The mixture composition was known to within ±0.0002 mole fraction. Ampoules were cooled to very low temperatures of about 220 K, pumped down and sealed. The sealed mixtures were then melted, cooled rapidly, and reheated. The rate of reheating was at an approximate rate of 8×10^{-5} K/s just before complete dissolution. The temperature at which the solid completely dissolved was recorded. The average of two or three independent measurements was taken as the solid-liquid equilibrium.

Source and Purity of Chemicals:
(1) 98%, Koch-Light Lab. Ltd., United Kingdom, was purified with concentrated sulfuric acid, followed by maleic anhydride, and then recrystallized to yield a sample of 99.86% purity (mass percent).
(2) Technical Grade, Leuna Werke, Federal Republic of Germany, was purified by super-rectification and then dried over molecular sieves to give a sample having a purity of 99.9% by mass.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±0.0002.

12. Solubility of Phenothiazine in Organic Solvents

12.1. Critical evaluation of experimental solubility data

The three earlier volumes in the IUPAC Solubility Data Series on solubilities of polycyclic aromatic hydrocarbons[1–3] contained very little solubility data for phenothiazine. Volume 59 (Ref. 3) contained phase diagram information for four binary systems, namely phenothiazine + phenoxazine, phenothiazine + thianthrene, phenothiazine + phenoxanthiin, and phenothiazine + dibenzo[b,e][1,4]dioxine. The experimental data will not be repeated here. The solubility information contained in Vol. 59 is listed so that readers will know what phenothiazine data are available in earlier volumes in the series.

There have been three studies that reported solubility data for phenothiazine in organic solvents after Vol. 59 was published in 1995. Hoover *et al.*[65] determined the solubility of phenothiazine in nine alkanes, 20 alkanols, one alkanediol, four dialkyl ethers, one cyclic ether, and three alkanenitriles at 298.15 K. They used the experimental solubility data to determine the Abraham model solute descriptors for phenothiazine. The calculated solute descriptors described observed solubility data to within ±0.094 log units. Saifullah *et al.*[66] reported the solubility of phenothiazine in tetrahydrofuran at 298.15 K as part of a computational study aimed at updating the Abraham model equation coefficients of tetrahydrofuran and 1,4-dioxane and extending the basic model to include ionic solute species. Finally, Ahmadian *et al.*[67] measured the solubility of phenothiazine in ethanol and 1,2-propanediol at 298.2, 308.2, 318.2, and 328.2 K.

There is only one solvent common to the three solubility studies. The mole fraction solubility of phenothiazine in ethanol of $x_1 = 0.00890$ reported by Hoover *et al.*[65] differs from the experimental value of $x_1 = 0.00876$ from the Ahmadian *et al.*[67] study by less than 2%.

The experimental solubility data for phenothiazine dissolved in the different organic solvents are given in Secs. 12.2–12.6.

12.2. Phenothiazine solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Hexane; C_6H_{14}; [110-54-3]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9994	0.000585

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Heptane; C_7H_{16}; [142-82-5]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9993	0.000696

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Octane; C_8H_{18}; [111-65-9]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9991	0.000858

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9989	0.001056

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9983	0.001661

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9990	0.000979

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9990	0.001027

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9984	0.001577

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Lancaster Synthesis, Ward Hill, Massachusetts, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9995	0.000532

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

12.3. Phenothiazine solubility data in ethers

Components: (1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	**Original Measurements:** [65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9742	0.02581

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	**Original Measurements:** [65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9881	0.01185

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	**Original Measurements:** [65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9886	0.01144

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9766	0.02339

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[66]M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8388	0.1612

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8974	0.1026

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9911	0.00890

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) Absolute, Aapar Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

12.4. Phenothiazine solubility data in alcohols

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Methanol; CH_4O; [67-56-1]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9949	0.00512

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Ethanol; C_2H_6O; [64-17-5]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Ethanol; C_2H_6O; [64-17-5]	[67]S. Ahmadian, V. Panahi-Azar, M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 4352 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
298.2	0.9912	0.00876
308.2	0.9900	0.0100
318.2	0.9878	0.0122
328.2	0.9855	0.0145

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 356 nm.

Source and Purity of Chemicals:
(1) 98%, Merck Chemicals, Germany, was recrystallized from propanone before use.
(2) 99.9%, Scharlau Chemie, Spain, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 K to ±0.6 K, the higher temperatures have greater uncertainty.
x_1: ±2.3% (relative uncertainty).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1-Propanol; C_3H_8O; [71-23-8]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9911	0.00885

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9940	0.00600

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9890	0.01099

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8+%, HPLC Grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9927	0.00732

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9947	0.00534

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9942	0.00583

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9866	0.01339

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [132-32-6]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9927	0.00726

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9910	0.00896

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9913	0.00871

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9844	0.01562

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)\ a}$	x_2^{b}	x_1^{c}
1.0000	0.9913	0.00866

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9927	0.00728

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Heptanol; $C_7H_{16}O$; [111-70-6]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9825	0.01754

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9814	0.01855

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9899	0.01009

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9802	0.01984

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9788	0.02119

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9981	0.00191

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[67]S. Ahmadian, V. Panahi-Azar, M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 4352 (2011).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
298.2	0.9958	0.00416
308.2	0.9946	0.00540
318.2	0.9934	0.00656
328.2	0.9923	0.00763
338.2	0.9915	0.00852

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Incubator, shaker, and an ultraviolet/visible spectrophotometer.
Solubility was determined by equilibrating an excess amount of solid naphthalene with the organic solvent using a shaker placed in an incubator equipped with a temperature controlling system. After an equilibration period of at least 48 h, the samples were withdrawn and filtered through hydrophobic Durapore filters (0.45 μm). The filtered sample was diluted quantitatively with methanol. Concentrations were determined by spectrophotmetric analysis at 356 nm.

Source and Purity of Chemicals:
(1) 98%, Merck Chemicals, Germany, was recrystallized from propanone before use.
(2) 99.9%, Scharlau Chemie, Spain, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.2 to ±0.6 K, the higher temperatures have greater uncertainty.
x_1: ±2.3% (relative uncertainty).

12.5. Phenothiazine solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	W. E. Acree, unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9195	0.08051

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9276	0.07241

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9288	0.07122

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9437	0.05625

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, used as received.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

12.6. Phenothiazine solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9883	0.01169

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Propanenitrile; C_3H_5N; [107-12-0]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9613	0.03872

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Butanenitrile; C_4H_7N; [109-74-0]	[65]K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9426	0.05741

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

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

Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 281 nm.

Source and Purity of Chemicals:

(1) 99%, Acros Organics, USA, was used as received.

(2) 99.7%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

13. Solubility of Pyrene in Organic Solvents

13.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained experimental solubility data for pyrene dissolved in nine saturated hydrocarbons (hexane, heptanes, octane, octadecane, cyclohexane, methylcyclohexane, cyclooctane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane), in five aromatic hydrocarbons (benzene, methylbenzene, 1,2-dimethylbenzene, 1,3-dimethylbenzene, and 1,4-dimethylbenzene), in three alkyl alkanoates (ethyl ethanoate, butyl ethanoate, and ethyl butanoate), in one dialkyl ether (1,1′-oxybisbutane) and one cyclic ether (1,4-dioxane), in four haloalkanes (tetrachloromethane, 1,2-dichloroethane, 1-chlorobutane, and 1,4-dichlorobutane), in 11 alkanols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 1-pentanol, 2-methyl-1-propanol, 2-methyl-1-propanol, 3-methyl-1-butanol, 1-octanol, and cyclopentanol) and one phenol (1-hydroxy-2-methylbenzene), and in three miscellaneous organic solvents (pyridine, dimethyl sulfoxide, and acetonitrile). Most of the experimental measurements were performed between 293 and 303 K. The compiled solubility data also included phase diagrams for binary pyrene + chrysene, pyrene + naphthalene, pyrene + octafluoronaphthalene, pyrene + 1,3-dinitrobenzene, pyrene + 1,4-dinitrobenzene, pyrene + 1,3,5-trinitrobenzene, pyrene + 1,2,3,5-tetranitrobenzene, pyrene + 2,4-dinitromethylbenzene, pyrene + 2,4-dinitrophenol, pyrene + 2,4,6-trinitromethylbenzene, pyrene + 2,4,6-trinitromethoxybenzene, pyrene + 2,4,6-trinitoraniline, pyrene + 2-chloro-1,3,5-trinitrobenzene, and pyrene + 3-methyl-2,4,6-trinitrophenol mixtures. Solubility data contained in Vol. 59 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for pyrene.

There have been several studies that reported solubility data for pyrene in organic solvents after Vol. 59 was published in 1995. Acree and co-workers[10,17,22,45,61,68–70] determined the solubility of pyrene in six alkanes (nonane, decane, undecane, dodecane, hexadecane, and squalane), in one aromatic hydrocarbon (ethylbenzene), in four alkyl alkanoates (methyl ethanoate, pentyl ethanoate, methyl butanoate, and dibutyl oxalate), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 2-methoxy-2-methylpropane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in three halogenated alkanes (1-chlorohexane, 1-chlorooctane, and chlorocyclohexane) and two halogenated benzenes (fluorobenzene and (trifluoromethyl)benzene), ten alkanols (2-methyl-2-propanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-decanol, 3,7-dimethyl-1-octanol, cyclohexanol, 1,2-ethanediol, and 2,2,2-trifluoroethanol), in five alkoxyalkanols (2-methoxyethanol, 2-methoxyethanol, 2-propoxyethanol, 2-butoxyethanol, and 3-methoxy-1-butanol), in two alkanones (butanone, cyclohexanone) and acetophenone, and in 15 different miscellaneous organic solvents (ethanenitrile, propanenitrile, butanenitrile, hexanedinitrile, benzonitrile, methyl acetoacetate, *N*-methylformamide, *N*,*N*-dimethylformamide, *N*,*N*-dimethylacetamide, benzeneamine, dimethyl sulfoxide, propylene carbonate, tributyl phosphate, morpholine, and ethanolamine). The experimental solubilities were measured at a single temperature of 299.15 K. Critical evaluations are not possible as there are no independent measurements for the phenanthrene–organic solvent systems studied by Acree and co-workers.[10,17,22,45,61,68–70]

Two research groups have studied the solubility behavior of pyrene as a function of temperature. Yu *et al.*[71] examined the solubility of pyrene in methylbenzene, ethyl ethanoate, tetrahydrofuran, methanol, ethanol, 1-propanol, 2-propanol and propanone at several temperatures between 293 and 333 K. In addition to reporting experimental solubilities, the authors provided a mathematical representation describing how the solubility varied with temperature based on the Apelblat model (see Eq. (3)) and calculated both the dissolution enthalpy and entropy of pyrene in the eight different solvents from plots of the natural logarithm of mole fraction solubility versus reciprocal absolute temperature. The authors' calculated curve-fit coefficients are given in Table 6, along with the root-mean-square deviations (RMSDs) for the respective mathematical representations. The root-mean-square deviation is defined by Eq. (9)

$$\mathrm{RMSD} = \frac{1}{N}\sum_{i=1}^{N}\left|\left(x_1^{\mathrm{calc}} - x_1^{\mathrm{exp}}\right)^2\right|^{1/2}, \tag{9}$$

where N is the number of experimental solubility measurements in an individual solute-solvent data set. The Apelblat model provided a very good mathematical description of the observed solubility behavior of pyrene as evidenced by the small RMSD values. It was also noted in the manuscript that the authors' experimental data at 298 K were in good

TABLE 6. Parameters of the Apelblat equation for describing the solubility of pyrene in various organic solvents

Solvent	*A*	*B*	*C*	RMSD
Methylbenzene[a]	−231.518	8511.8	35.145	0.001396
Ethyl ethanoate[a]	−295.480	11362.5	44.605	0.000970
Methanol[a]	−21.919	−1578.6	3.630	0.000041
Ethanol[a]	−147.196	4300.3	22.292	0.000042
1-Propanol[a]	−180.557	5549.2	27.463	0.000067
2-Propanol[a]	−190.169	5835.4	28.929	0.000049
Tetrahydrofuran[a]	−84.110	2415.7	12.995	0.001421
Propanone[a]	−184.688	6062.2	28.246	0.000367
Hexane[b]	44.139	−4126.7	−6.112	0.000231
Methylcyclohexane[b]	34.845	−4126.4	−4.404	0.000440
Benzene[b]	17.063	−4126.8	−1.029	0.000753
Ethylbenzene[b]	15.133	−4126.8	−0.670	0.003241
1-Hexanol[b]	46.292	−4126.1	−6.436	0.000224
Octane[c]	42.018	−4126.2	−5.657	0.000188
2,2,4-Trimethylpentane[c]	36.658	−4126.3	−4.837	0.000133
1,4-Dimethylbenzene[c]	48.383	−4126.0	−6.491	0.000298
1-Octanol[c]	41.770	−4126.2	−5.550	0.000207

[a] Numerical values of the coefficients and the percent mean relative deviations were taken from Yu *et al.*[71]

[b] Numerical values of the coefficients and the percent mean relative deviations were taken from Ali and Al-Rashed.[73]

[c] Numerical values of the coefficients and the percent mean relative deviations were taken from Ali.[74]

agreement with previously published by Powell *et al.*[72] (which is given in Vol. 59 of the IUPAC Solubility Data Series[3]). It is further noted that the measured solubility of pyrene in tetrahydrofuran at 298.75 K, $x_1 = 0.1427$, is in good agreement with the value of $x_1 = 0.1402$ determined by Acree and Abraham[10] for 299.15 K.

Ali and Al-Rashed[73] studied the solubility of pyrene in both single solvents and in multi-component solvent mixtures containing hexane, methylcyclohexane, benzene, methylbenzene, and 1-hexanol over the temperature range from 293 to 318 K. The measured mole fraction solubilities were used to test the descriptive and predictive abilities of the Wilson, Combined NIBS/Redlich-Kister, UNIQAC, Non-Random Two Liquid solution models. The models were found to describe the observed solubility behavior of pyrene in quaternary benzene + hexane + 1-hexanol + methylcyclohexane, quaternary ethylbenzene + hexane + 1-hexanol + methylcyclohexane and pentinary benzene + ethylbenzene + hexane + 1-hexanol + methylcyclohexane to within a deviation of 15% or less using interaction parameters calculated from the measured pyrene solubilities in the contributing sub-binary solvent systems. The authors further noted that plots of the natural logarithm of the mole fraction solubility versus reciprocal temperature (e.g., ln x_1 versus $1/T$) resulted in linear plots having squared correlation coefficients of $R^2 = 0.96$ to $R^2 = 0.99$ as would be expected for internally consistent experimental solubility data. Ali[74] had previously measured the solubility of pyrene in octane, 2,2,4-trimethylpentane, 1,4-dimethylbenzene and 1-octanol. Also tabulated in Table 6 are the equation coefficients for the Apelblat equation and the corresponding RMSDs for these latter nine pyrene–organic solvent systems.

The experimental solubility data for pyrene in the different organic solvents are given in Secs. 13.2–13.10.

13.2. Pyrene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Hexane; C_6H_{14}; [110-54-3]	[73] S. H. Ali and O. A. Al-Rashed, Fluid Phase Equilib. **281**, 133 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9900	0.0100
298	0.9896	0.0104
303	0.9877	0.0123
308	0.9871	0.0129
313	0.9843	0.0157
318	0.9819	0.0181

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.

Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, chemical source not given, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Octane; C_8H_{18}; [111-65-9]	[74]S. H. Ali, Fluid Phase Equilib. **264**, 29 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9844	0.0156
298	0.9831	0.0169
303	0.9805	0.0195
308	0.9781	0.0219
313	0.9741	0.0259
318	0.9710	0.0290

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, Fluka, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Nonane; C_9H_{20}; [111-84-2]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compds. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9832	0.01678

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[45]L. E. Roy, C. E. Hernández and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9806	0.01936

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ethanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Undecane; $C_{11}H_{24}$; [1120-21-4]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9779	0.02213

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in undecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ethanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Dodecane; $C_{12}H_{26}$; [112-40-3]	[17]M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9756	0.02439

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Experimental values were reported as the logarithm of the solute's molar solubility in dodecane divided by the molar solubility in water. Mole fraction solubilities were provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ethanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9657	0.03431

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ethanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Octacosane; $C_{28}H_{58}$; [630-02-4]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
333.91	1.0000	0.0000
333.64	0.8810	0.1190
333.54	0.7577	0.2423
344.00	0.6993	0.3007
370.57	0.5965	0.4035
387.15	0.4994	0.5006
398.87	0.4001	0.5999
407.36	0.2998	0.7002
414.52	0.2000	0.8000
418.36	0.1001	0.8999
422.65	0.0000	1.0000

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of pyrene and octacosane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\text{K} = 330.6$ and eutectic mole fraction of pyrene of $x_1 = 0.218$.

Auxiliary Information

Method/Apparatus/Procedure:
Differential scanning calorimeter.
The phase diagram was determined using a differential scanning calorimeter. Measurements were performed at a constant fixed scanning rate of 0.5 K/min.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.
(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:
Temperature: Authors state a global accuracy of ±1% regarding their measurements.
x_1: ± 0.0002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[73]S. H. Ali and O. A. Al-Rashed, Fluid Phase Equilib. **281**, 133 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9850	0.0150
298	0.9842	0.0158
303	0.9814	0.0186
308	0.9763	0.0237
313	0.9723	0.0277
318	0.9711	0.0289

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, chemical source not given, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[74]S. H. Ali, Fluid Phase Equilib. **264**, 29 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9927	0.0073
298	0.9914	0.0086
303	0.9896	0.0104
308	0.9880	0.0120
313	0.9865	0.0135
318	0.9854	0.0146

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, Fluka, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$	x_2	x_1
1.0000	0.9622	0.03776

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Squalane; $C_{30}H_{62}$; [111-01-3]	[15]A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
345.75	0.8480	0.1520
361.35	0.7971	0.2029
380.15	0.6984	0.3016
392.65	0.5943	0.4057
400.15	0.4996	0.5004
405.35	0.4005	0.5995
410.45	0.2999	0.7001
413.85	0.2004	0.7996
415.35	0.1491	0.8509
416.95	0.1070	0.8930
419.45	0.0505	0.9495

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

The authors employed a SSF to describe the activity coefficients of pyrene and squalane calculated from the solid-liquid equilibrium data. The SSF model gave a calculated eutectic temperature of $T/\mathrm{K} = 243.1$ and eutectic mole fraction of pyrene of $x_1 = 0.006$.

Auxiliary Information

Method/Apparatus/Procedure:

Simple thermal analysis device constructed in the authors' laboratory, and a high precision platinum-resistance thermometer.

The phase diagram was determined using a simple thermal device. A sample of known composition was placed in a thermostatted glass tube, melted and then slowly cooled at a rate of about 1 K/min. The temperature of the sample was measured with a high precision platinum-resistance thermometer. The crystallization temperature was obtained from a plot of the cooling curve versus time. Each measurement was repeated three times.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were given in the paper.

(2) 99%, Aldrich Chemical Company, purification details were not given in the paper.

Estimated Error:

Temperature: Authors state a global accuracy of ±1% regarding their measurements.

x_1: ± 0.0002 (estimated by compiler).

13.3. Pyrene solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Benzene; C_6H_6; [71-43-2]	[73]S. H. Ali and O. A. Al-Rashed, Fluid Phase Equilib. **281**, 133 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9416	0.0584
298	0.9290	0.0710
303	0.9151	0.0849
308	0.8936	0.1064
313	0.8687	0.1313
318	0.8383	0.1617

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.

Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:

(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.

(2) 99.9+%, chemical source not given, no purification details were provided in the paper.

Estimated Error:

Temperature: ±0.1 K.

x_1: <3.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Methylbenzene; C_7H_8; [108-88-3]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.35	0.9389	0.0611
303.75	0.9243	0.0757
308.65	0.9134	0.0866
313.55	0.9050	0.0950
318.45	0.8900	0.1100
323.35	0.8780	0.1220
328.15	0.8600	0.1400
333.15	0.8355	0.1645

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, oven and electronic balance.

Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:

(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.

(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: <1.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Ethylbenzene; C_8H_{10}; [100-41-4]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9358	0.06424

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Ethylbenzene; C_8H_{10}; [100-41-4]	[73]S. H. Ali and O. A. Al-Rashed, Fluid Phase Equilib. **281**, 133 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
293	0.9349	0.0651
298	0.9224	0.0776
303	0.9056	0.0944
308	0.8776	0.1224
313	0.8353	0.1647
318	0.8290	0.1710

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, chemical source not given, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]	[74]S. H. Ali, Fluid Phase Equilib. **264**, 29 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
293	0.9223	0.0777
298	0.9137	0.0863
303	0.9024	0.0976
308	0.8907	0.1093
313	0.8764	0.1236
318	0.8633	0.1367

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, Fluka, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

13.4. Pyrene solubility data in esters

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9670	0.03296

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
295.35	0.9634	0.0366
298.75	0.9602	0.0398
303.75	0.9544	0.0456
308.65	0.9486	0.0514
313.45	0.9418	0.0582
318.45	0.9349	0.0651
323.35	0.9264	0.0736
328.15	0.9114	0.0886
333.15	0.8981	0.1019

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, oven and electronic balance.
Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:
(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.
(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: <1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9292	0.07077

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Methyl butanoate; $C_5H_{10}O_2$; [623-42-7]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9463	0.05367

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Dibutyl oxalate; $C_{10}H_{18}O_4$; [2050-60-4]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8891	0.1109

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

13.5. Pyrene solubility data in ethers

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9713	0.02865

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9798	0.02015

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9757	0.02432

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The published value was given as molar solubility of pyrene in 2-methoxy-2-methylpropane (also called methyl *tert*-butyl ether). The mole fraction solubility was provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8598	0.1402

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.35	0.8653	0.1347
298.75	0.8573	0.1427
303.75	0.8484	0.1516
308.65	0.8345	0.1655
313.45	0.8199	0.1801
318.45	0.8005	0.1995
323.35	0.7864	0.2136
328.15	0.7668	0.2332
333.15	0.7477	0.2523

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, oven and electronic balance.
Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:
(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.
(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: <5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9232	0.07676

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The solubility was re-measured because an earlier published value[72] was out of line with observed pyrene solubility data for other ethers. The authors suspected that a twofold dilution had been missed when converting the earlier set of measured absorbances to mole fraction solubilities.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

13.6. Pyrene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9244	0.07557

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9140	0.08601

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9337	0.06625

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Fluorobenzene; C_6H_5F; [462-06-6]	[22]M. H. Abraham, W. E. Acree, Jr., A. J. Leo, and D. Hoekman, New J. Chem. **33**, 1685 (2009).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9383	0.06168

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The experimental value was reported as the logarithm of pyrene's molar solubility in fluorobenzene dissolved by the solute's molar solubility in water. Experimental mole fraction solubility was obtained from the authors.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) (Trifluoromethyl)benzene; $C_7H_5F_3$; [98-08-8]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9624	0.03756

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

13.7. Pyrene solubility data in alcohols

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Methanol; CH_4O; [67-56-1]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
293.95	0.9987	0.00127
298.35	0.9985	0.00149
303.85	0.9983	0.00170
308.65	0.9980	0.00202
313.35	0.9978	0.00223
318.35	0.9974	0.00262
323.35	0.9971	0.00288
328.15	0.9966	0.00341
333.15	0.9962	0.00379

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, oven and electronic balance.

Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K, and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:

(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.

(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: <5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Ethanol; C_2H_6O; [64-17-5]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
299.55	0.9971	0.00294
298.85	0.9968	0.00321
303.75	0.9964	0.00363
308.75	0.9958	0.00424
313.55	0.9952	0.00479
318.45	0.9946	0.00536
323.45	0.9937	0.00628
328.15	0.9928	0.00720
333.15	0.9918	0.00820

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, oven and electronic balance.

Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K, and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:

(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.

(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: <1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.25	0.9973	0.00268
290.05	0.9966	0.00342
296.95	0.9960	0.00404
303.75	0.9950	0.00499
310.85	0.9939	0.00607
317.55	0.9924	0.00761
323.55	0.9907	0.00930
331.35	0.9882	0.01179

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, oven and electronic balance.

Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:

(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.

(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: <4% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [67-63-0]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.35	0.9980	0.00201
290.05	0.9976	0.00242
296.95	0.9971	0.00292
300.85	0.9965	0.00350
307.85	0.9958	0.00420
314.55	0.9947	0.00530
321.45	0.9933	0.00667
328.15	0.9916	0.00835
333.15	0.9901	0.00989

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, oven and electronic balance.
Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:
(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.
(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: <5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9969	0.003134

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[68]M. E. R. McHale, A.-S. M. Horton, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Vela, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1522 (1996).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9936	0.00640

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before being fractionally distilled.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9938	0.00617

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9873	0.01273

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[73]S. H. Ali and O. A. Al-Rashed, Fluid Phase Equilib. **281**, 133 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2^{a}	x_1^{b}
293	0.9863	0.0137
298	0.9857	0.0143
303	0.9841	0.0159
308	0.9817	0.0183
313	0.9788	0.0212
318	0.9763	0.0237

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, chemical source not given, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[70]M. E. R. McHale, K. A. Fletcher, K. S. Coym, W. E. Acree, Jr., V. G. Varanasi, and S. W. Campbell, Phys. Chem. Liq. **34**, 103 (1997).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9921	0.00789

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9938	0.00621

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9831	0.01694

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[74]S. H. Ali, Fluid Phase Equilib. **264**, 29 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9781	0.0219
298	0.9759	0.0241
303	0.9715	0.0285
308	0.9667	0.0333
313	0.9634	0.0366
318	0.9589	0.0411

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, gas chromatograph equipped with a flame ionization detector and an uv/visible spectrophotometer.
Saturated solutions were prepared by placing excess solute in glass bottles containing the solvent. Samples were equilibrated in a constant temperature with shaking for at least three days, followed by a three-day period in which the solid was allowed to settle to the bottom of the container. Aliquots were transferred to tared volumetric flasks, weighed and then diluted with the solvent for spectrophotometric analysis. Concentrations of the dilute solutions were determined from absorbance versus concentration curves based on absorbance measurements for standard solutions of known concentration. The spectrophotometric results were verified by gas chromatographic analyses.

Source and Purity of Chemicals:
(1) 97%, Fluka, recrystallized several times from methanol to yield a sample of 99% purity.
(2) 99.9+%, Baker Chemical Company, USA, no purification details were provided in the paper.

Estimated Error:
Temperature: ±0.1 K.
x_1: <3.0% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9714	0.02859

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

The published value was given as molar solubility of pyrene in 1-decanol. The mole fraction solubility was provided by the authors of the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 3,7-Dimethyl-1-octanol; $C_{10}H_{22}O$; [106-21-8]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9831	0.01694

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[68]M. E. R. McHale, A.-S. M. Horton, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Vela, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1522 (1996).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9903	0.00965

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9995	0.000519

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9995	0.000467

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

13.8. Pyrene solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9828	0.01717

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5+%, anhydrous, Aldrich Chemical Company, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9695	0.03046

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over anhydrous sodium sulfate molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9660	0.03400

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9621	0.03790

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[69]M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9746	0.02541

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.3% (relative error).

13.9. Pyrene solubility data in ketones

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Propanone; C_3H_6O; [67-64-1]	[71]Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.35	0.9697	0.0303
299.05	0.9668	0.0332
303.75	0.9618	0.0382
308.65	0.9564	0.0436
313.55	0.9498	0.0502
318.45	0.9433	0.0567
323.35	0.9334	0.0666

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the polycyclic aromatic hydrocarbon (component 1).

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, oven and electronic balance.
Saturated solutions were prepared by placing excess solute in a cylindrical double-jacketed glass vial. The solution was equilibrated at constant temperature with continuous stirring for at least 4 h. The stirring was discontinued and the solution was allowed to stand for 3 h. An aliquot of the upper clear solution was removed, filtered through a 0.45 μm membrane, and transferred to a tared double dish. The double dish and contents were quickly weighed. The solvent in the double dish was evaporated, dried at 325 K and then reweighed. The solubility was determined from the mass of the solid residue and the mass of the sample analyzed. Measurements were performed in triplicate.

Source and Purity of Chemicals:
(1) 99%, Alfa Aesar Reagent Company, was recrystallized twice from propanone.
(2) 99.9+%, Tianjin Kemel Chemical, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) 2-Butanone; C_4H_8O; [78-93-3]	[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9325	0.06752

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.5+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.8900	0.1100

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Acetophenone; C_8H_8O; [98-86-2]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8848	0.1152

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

13.10. Pyrene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9939	0.00614

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Propanenitrile; C_3H_5N; [107-12-0]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables: T/K = 299.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9744	0.02562

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Butanenitrile; C_4H_7N; [109-74-0]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9558	0.04417

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Hexanedinitrile; $C_6H_8N_2$; [111-69-3]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9747	0.02528

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Benzonitrile; C_7H_5N; [100-47-0]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.8985	0.1015

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Methyl acetoacetate; $C_5H_8O_3$; [105-45-3]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9689	0.03106

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) *N*-Methylformamide; C_2H_5NO; [123-39-7]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9935	0.006512

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9116	0.08844

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:
[45]L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).

Variables:
T/K = 299.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8625	0.1375

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) Benzenamine; C_6H_7N; [62-53-3]

Original Measurements:
[61]C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).

Variables:
T/K = 299.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9660	0.03398

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) ACS Reagent Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]

Original Measurements:
[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).

Variables:
T/K = 299.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9665	0.03354

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9815	0.01847

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Tributyl phosphate; $C_{12}H_{27}O_4P$; [126-73-8]	[10]W. E. Acree, Jr. and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8707	0.1293

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Morpholine; C_4H_9NO; [110-91-8]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9178	0.08218

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Ethanolamine; C_2H_7NO; [141-43-5]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 299.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9980	0.001953

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

14. Solubility of Thianthrene in Organic Solvents

14.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained only experimental solubility data for thianthrene dissolved in eight saturated hydrocarbon solutes, namely hexane, heptanes, octane, cyclohexane, methylcyclohexane, cyclooctane, and 2,2,4-trimethylpentane. Experimental measurements were performed at a single temperature of 298.15 K. The compiled solubility data also included phase diagram information for binary thianthrene + phenanthrene, thianthrene + phenothiazine, thianthrene + phenoxanthiin, and thianthrene + phenoxazine mixtures. Solubility data contained in Vol. 59 will not be republished here. The listing above is provided so that readers will know what solubility data are available in the earlier volume for thianthrene.

There have been two studies that reported solubility data for thianthrene in organic solvents after Vol. 59 was published in 1995. Fletcher *et al.*[75] determined the solubility of thianthrene in 21 different organic solvents containing hydroxyl-, ether- or *tert*-butyl functional groups. The measured solubility data were used to test the applications and limitations of predictive expressions derived from Mobile Order theory. Stovall *et al.*[76] subsequently determined solubilities in nonane, decane, undecane, hexadecane, 1,1′-oxybisethane, 2,2′-oxybispropane, 1,4-dioxane, 1-decanol, ethylene glycol, and ethanenitrile to increase the experimental data available for determining the numerical values of the Abraham model solute descriptors of thianthrene. The calculated solute descriptors derived from the experimental solubility data provided a very good mathematical description of the solubility behavior of thianthrene in organic solvents, with an average absolute deviation between calculated and experimental values on the order of ±0.12 log units. Both research groups performed the solubility measurements at the single temperature of 298.15 K. Critical evaluations are not possible as there are no independent measurements for the thianthrene–organic solvent systems studied by Fletcher *et al.*[75] and Stovall *et al.*[76]

The solubility data for thianthrene are given in Secs. 14.2–14.5.

14.2. Thianthrene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Nonane; C_9H_{20}; [111-84-2]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9955	0.004465

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9950	0.004980

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Undecane; $C_{11}H_{24}$; [1120-21-4]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9944	0.005636

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9918	0.008166

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9934	0.00658

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

14.3. Thianthrene solubility data in ethers

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9916	0.008363

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9936	0.006376

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9903	0.00970

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9906	0.00939

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9757	0.02431

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

14.4. Thianthrene solubility data in alcohols

Components:
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9995	0.000472

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9990	0.001038

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3]
(2) 1-Propanol; C_3H_6O; [71-23-8]

Original Measurements:
[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
1.0000	0.9984	0.00162

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Propanol; C_3H_6O; [67-63-0]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9990	0.001007

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9977	0.00227

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9983	0.00166

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9985	0.00149

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9969	0.00308

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9979	0.00208

$^a x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^b x_2$: mole fraction of component 2 in the saturated solution.
$^c x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9976	0.00243

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9976	0.00235

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^b	x_1^c
1.0000	0.9961	0.00390

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9971	0.00287

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9977	0.00230

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9950	0.00501

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9945	0.00553

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9958	0.00415

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-4]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9930	0.007021

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]	[75]K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9959	0.00408

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9987	0.001278

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

14.5. Thianthrene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Thianthrene; $C_{12}H_8S_2$; [92-85-3] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9986	0.001364

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 255 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

15. Solubility of Xanthene in Organic Solvents

15.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained experimental solubility data for xanthene in two saturated hydrocarbons (cyclohexane and decahydronaphthalene), in two aromatic hydrocarbons (benzene and 1,2,3,4-tetrahydronaphthalene), and in two miscellaneous organic solvents (pyridine and thiophene). All six systems included measurements at several temperatures covering a 40 to 50 K range. Solubility data contained in Vol. 59 are not included in the present volume. The above listing is provided so that readers will know what data are available in the earlier volume for xanthene.

There have been three studies that reported solubility data for xanthene in organic solvents after Vol. 59 was published in 1995. Monárrez *et al.*[77] determined the solubility of xanthene in 34 different organic solvents containing hydroxyl-, ether-, chloro-, cyano- or *tert*-butyl functional groups. The measured solubility data were used to test the applications and limitations of predictive expressions derived from Mobile Order theory. Stovall *et al.*[76] subsequently determined solubilities in undecane, 1,1′-oxybisethane and 2,2′-oxybispropane to increase the experimental data available for determining the numerical values of the Abraham model solute descriptors of xanthene. The calculated solute descriptors derived from the experimental solubility data provided a very good mathematical description of the solubility behavior of xanthene in organic solvents, with an average absolute deviation between calculated and experimental values being on the order of ±0.09 log units. Saifullah *et al.*[66] later reported the solubility of xanthene in both tetrahydrofuran and 1,4-dioxane at 298.15 K as part of a computational study aimed at updating the Abraham model equation coefficients of tetrahydrofuran and 1,4-dioxane and extending the basic model to include ionic solute species. All three research groups performed the solubility measurements at the single temperature of 298.15 K. Critical evaluations are not possible as there are no independent measurements for the xanthene–organic solvent systems studied by Monárrez *et al.*,[77] Stovall *et al.*,[76] and Saifullah *et al.*[66]

The experimental solubility data for xanthene in the different organic solvents are in Secs. 15.2–15.7.

15.2. Xanthene solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Hexane; C_6H_{14}; [110-54-3]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9705	0.02949

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Heptane; C_7H_{16}; [142-82-5]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9646	0.03543

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Octane; C_8H_{18}; [111-65-9]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9602	0.03976

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Nonane; C_9H_{20}; [111-84-2]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9569	0.04306

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9539	0.04610

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, TCI America, Portland, OR, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Undecane; $C_{11}H_{24}$; [1120-21-4]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 111 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9530	0.04704

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Acros Organics, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9316	0.06835

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9580	0.04203

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9572	0.04275

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Cyclooctane; C_8H_{16}; [292-64-8]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9459	0.05414

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Lancaster Synthesis, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9755	0.02451

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

15.3. Xanthene solubility data in ethers

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 111 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9165	0.08353

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[76]D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 111 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9447	0.05531

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9169	0.08310

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9215	0.07846

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[66]M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8140	0.1860

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[66]M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8498	0.1502

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

15.4. Xanthene solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Tetrachloromethane; CCl_4; [56-23-5]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8763	0.1237

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.5+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.8451	0.1549

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

15.5. Xanthene solubility data in alcohols

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Methanol; CH_4O; [67-56-1]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9955	0.004455

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.9+%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Ethanol; C_2H_6O; [64-17-5]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9938	0.006231

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Propanol; C_3H_8O; [71-23-8]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9883	0.01166

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Propanol; C_3H_8O; [67-63-0]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9914	0.008643

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9824	0.01756

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99.8+%, HPLC Grade, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9875	0.01254

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9892	0.01077

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9889	0.01112

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9779	0.02212

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9823	0.01766

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9837	0.01633

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9805	0.01946

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9717	0.02831

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9803	0.01969

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9824	0.01762

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9666	0.03340

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9620	0.03800

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9547	0.04528

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Cyclopentanol; $C_5H_{10}O$; [96-41-3]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9711	0.02886

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

15.6. Xanthene solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	W. E. Acree, unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9570	0.04299

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9435	0.05649

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the solution.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9471	0.05285

$^{a}x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^{b}x_2$: mole fraction of component 2 in the saturated solution.
$^{c}x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9471	0.05288

$^{a}x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^{b}x_2$: mole fraction of component 2 in the saturated solution.
$^{c}x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA, stored over anhydrous sodium sulfate and molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

15.7. Xanthene solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Xanthene; $C_{13}H_{10}O$; [92-83-1] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[77]C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
1.0000	0.9803	0.01970

$^{a}x_2^{(s)}$: initial mole fraction of component 2 in the solution.
$^{b}x_2$: mole fraction of component 2 in the saturated solution.
$^{c}x_1$: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

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

Excess solute and solvent were 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 were transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:

(1) 98%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized several times from anhydrous methanol.

(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

16. References

[1] *Polycyclic Aromatic Hydrocarbons in Pure and Binary Solvent Mixtures*, edited by W. E. Acree, Jr., IUPAC Solubility Data Series, Vol. 54 (Oxford University Press, London, 1994).

[2] *Polycyclic Aromatic Hydrocarbons: Binary Nonaqueous Systems. Part I. Solutes A-E*, edited by W. E. Acree, Jr., IUPAC Solubility Data Series, Vol. 58 (Oxford University Press, London, 1995).

[3] W. E. Acree, Jr., *Polycyclic Aromatic Hydrocarbons: Binary Nonaqueous Systems. Part 2. Solutes F-Z*, IUPAC Solubility Data Series, Vol. 59 (Oxford University Press, London, 1995).

[4] W. E. Acree, Jr., J. Phys. Chem. Ref. Data **42**, 013103 (2013).

[5] W. E. Acree, Jr., J. Phys. Chem. Ref. Data **42**, 013104 (2013).

[6] J. M. Prausnitz, *Molecular Thermodynamics of Fluid-Phase Equilibria* (Prentice-Hall, Englewood Cliffs, NJ, 1969).

[7] H. Buchowski, A. Ksiazczak, and S. J. Pietrzyk, J. Phys. Chem. **84**, 975 (1980).

[8] H. Buchowski and A. Khiat, Fluid Phase Equilib. **25**, 273 (1986).

[9] K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1537 (1999).

[10] W. E. Acree, Jr and M. H. Abraham, Fluid Phase Equilib. **201**, 245 (2002).

[11] E. McLaughlin and H. A. Zainal, J. Chem. Soc. 3854 (1960).

[12] P. B. Choi, C. P. Williams, K. G. Buehring, and E. McLaughlin, J. Chem. Eng. Data **30**, 403 (1985).

[13] I. Kotula and B. Marciniak, J. Chem. Eng. Data **46**, 783 (2001).

[14] F. He and P. Liu, J. Chem. Eng. Data **52**, 2536 (2007).

[15] A. Aoulmi, M. Bouroukba, R. Solimando, and M. Rogalski, Fluid Phase Equilib. **110**, 283 (1995).

[16] L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 105 (1999).

[17] M. H. Abraham and W. E. Acree, Jr., New J. Chem. **28**, 1538 (2004).

[18] L. Alcazar, A. Blanco, R. Cano, L. Fisher, M. Nau, L. Sidransky, and W. E. Acree, Jr., J. Chem. Eng. Data **53**, 201 (2008).

[19] M. Carrillo, M. Corella, K. Wolcott, K. R. Bowen, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 270 (2007).

[20] J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).

[21] K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).

[22] M. H. Abraham, W. E. Acree, Jr., A. J. Leo, and D. Hoekman, New J. Chem. **33**, 1685 (2009).

[23] K. M. De Fina, T. T. Van, A. Ibarra, E. Hamilton, J. Martinez, A. Valdez, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 249 (2001).

[24] J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).

[25] C. I. Monárrez, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1341 (2003).

[26] J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, Jr., V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).

[27] J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, P. Otero, M. Jayasekera, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1270 (1995).

[28] W. E. Acree, Jr. and M. H. Abraham, Can. J. Chem. **79**, 1466 (2001).

[29] C. E. Hernández, L. E. Roy, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 677 (1999).

[30] C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Jackson, G. Brown, and W. E. Acree, Jr., Chem. Eng. Commun. **169**, 137 (1998).

[31] C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Jackson, G. Brown, T. L. Borders, J. T. Sanders, and W. E. Acree, Jr., Phys. Chem. Liq. **36**, 257 (1998).

[32] M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).

[33] C. E. Hernández, L. E. Roy, G. D. Reddy, T. L. Borders, J. T. Sanders, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 31 (1998).

[34] A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).

[35] Z. Lisicki and M. E. Jamróz, J. Chem. Thermodyn. **32**, 1335 (2000).

[36] K. M. De Fina, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1589 (1999).

[37] L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).

[38] A. C. Mengarelli, S. B. Bottini, and E. A. Brignole, J. Chem. Eng. Data **40**, 746 (1995).

[39] J. E. Coon, W. B. Sediawan, J. E. Auwaerter, and E. McLauglin, J. Solution Chem. **17**, 519 (1988).

[40] U. Domanska, F. R. Broves, Jr., and E. McLaughlin, J. Chem. Eng. Data **38**, 88 (1993).

[41] Y. Wei, L. Dang, Z. Zhang, W. Cui, and H. Wei, J. Chem. Eng. Data **57**, 1279 (2012).

[42] S. L. Hafsaoui and R. Mahmoud, J. Therm Anal. Calorim. **88**, 565 (2007).

[43] L. F. Ramirez-Verduzco, A. Rojas-Aguilar, J. A. De los Reyes, J. A. Munoz-Arroyo, and F. Murrieta-Guevara, J. Chem. Eng. Data **52**, 2212 (2007).

[44] C. E. Hernández and W. E. Acree, Jr., Can. J. Chem. **76**, 1312 (1998).

[45] L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Polycyclic Aromat. Compd. **13**, 205 (1999).

[46] R. Pinal, P. S. C. Rao, L. S. Lee, P. V. Cline, and S. H. Yalkowsky, Environ. Sci. Technol. **24**, 639 (1990).

[47] M. M. Miller, S. P. Waskik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

[48] C. I. Monárrez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **40**, 581 (2002).

[49] D. M. Stovall, K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Polycyclic Aromat. Compd. **25**, 313 (2005).

[50] Z. Zou, L. Dang, P. Liu, and H. Wei, J. Chem. Eng. Data **52**, 1501 (2007).

[51] Y. Han and Z. Wang, J. Chem. Eng. Data **54**, 148 (2009).

[52] T.-B. Cui, T.-L. Luo, C. Zhang, Z.-B. Mao, and G.-J. Liu, J. Chem. Eng. Data **54**, 1065 (2009).

[53] Q.-S. Li, Z.-M. Yi, M.-G. Su, and X.-F. Sun, J. Chem. Eng. Data **53**, 2701 (2008).

[54] P. M. Ghogomu, R. Rakolosaona, M. Bouroukba, D. Petitjean, N. Hubert, and M. Dirand, Mol. Cryst. Liq. Cryst. **408**, 103 (2004).

[55] T. Tsuji, K. Sue, T. Hiaki, and N. Itoh, Fluid Phase Equilib. **257**, 183 (2007).

[56] B. L. Sharma, R. Kant, R. Sharma, and S. Tandon, Mater. Chem. Phys. **82**, 216 (2003).

[57] D. Wei and K. Jin, J. Chem. Thermodyn. **41**, 145 (2009).

[58] U. S. Rai and R. N. Rai, Asian J. Chem. **10**, 421 (1998).

[59] A. Shayanfar, S. Soltani, F. Jabbaribar, A. A. Hamidi, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **53**, 574 (2008).

[60] A. F. Lagalante, A. Abdulagatov, and T. J. Bruno, J. Chem. Eng. Data **47**, 47 (2002).

[61] C. E. Hernández, K. M. De Fina, L. E. Roy, T. L. Sharp, and W. E. Acree, Jr., Can. J. Chem. **77**, 1465 (1999).

[62] M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).

[63] M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, Ind. Eng. Chem. Res. **49**, 6238 (2010).

[64] Y. Bakhbakhi, P. Charpentier, and S. Rohani, Can. J. Chem. Eng. **83**, 267 (2005).

[65] K. R. Hoover, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **44**, 367 (2006).

[66] M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).

[67] S. Ahmadian, V. Panahi-Azar, M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 4352 (2011).

[68] M. E. R. McHale, A.-S. M. Horton, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Vela, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1522 (1996).

[69] M. E. R. McHale, K. S. Coym, K. A. Fletcher, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 511 (1997).

[70] M. E. R. McHale, K. A. Fletcher, K. S. Coym, W. E. Acree, Jr., V. G. Varanasi, and S. W. Campbell, Phys. Chem. Liq. **34**, 103 (1997).

[71] Q. Yu, X. Ma, and L. Xu, Fluid Phase Equilib. **319**, 5 (2012).

[72] J. R. Powell, D. Voisinet, A. Salazar, and W. E. Acree, Jr., Phys. Chem. Liq. **28**, 269 (1994).

[73] S. H. Ali and O. A. Al-Rashed, Fluid Phase Equilib. **281**, 133 (2009).

[74] S. H. Ali, Fluid Phase Equilib. **264**, 29 (2008).

[75] K. A. Fletcher, M. E. R. McHale, J. R. Powell, K. S. Coym, and W. E. Acree, Jr., Phys. Chem. Liq. **34**, 41 (1997).

[76] D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **232**, 113 (2005).

[77] C. I. Monárrez, D. M. Stovall, J. H. Woo, P. Taylor, and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 703 (2002).