IUPAC-NIST Solubility Data Series. 98. Solubility of Polycyclic Aromatic Hydrocarbons in Pure and Organic Solvent Mixtures: Revised and Updated. Part 1. Binary Solvent Mixtures

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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 binary organic solvent mixtures. Published solubility data for anthracene, naphthalene, phenanthrene, phenothiazine, and pyrene that appeared in the primary literature between 1995 to the end of 2011 are compiled and critically evaluated. Experimental solubility data for 360 different solute-binary solvent systems are included in the volume. 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/10.1063/1.4772674]

Key words: alcohols; alkanes; alkanenitriles; alkoxyalcohols; alkyl ethanoates; anthracene; binary solvent mixtures; chloroalkanes; dialkyl ethers; naphthalene; phenanthrene; phenothia.zine; polycyclic aromatic hydrocarbons; pyrene; solubility.

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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 in still in press at the time.

This paper is the first part of a planned three-part volume that will update the three earlier volumes on PAH and PAHaC solubilities. Part 1 is 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. To conserve space, data from the earlier volumes will not be repeated here. Part 2 will deal with solubilities of PAHs and PAHaCs dissolved in ternary solvent mixtures, while Part 3 will focus on the organic mono-solvents (neat organic solvents).

1.2. Concentration units for nonelectrolyte solutions

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

$$c_i = [i] = \frac{n_i}{V} \quad \text{SI base units: mol dm}^{-3}, \tag{1}$$

(3) mole fraction

$$x_i = \frac{n_i}{n_1 + n_2 + \ldots. + n_i + \ldots.}, \tag{2}$$

or (4) volume fraction

$$\phi_i = \frac{n_i V_i}{n_1 V_1 + n_2 V_2 + \ldots. + n_i V_i + \ldots.}. \tag{3}$$

Strictly speaking, the true volume of a real solution is not equal to the sum of the volumes of the individual components but is the fraction sum of partial volumes, which for a ternary solution is $V = x_1 V_1 + x_2 V_2 + x_3 V_3$. For purposes of this study, volume fractions are defined in terms of the molar volumes of the pure unmixed components, $V_{m,i}$ (molar mass of component i divided by density of component i),

$$\phi_i = \frac{n_i V_{m,i}}{n_1 V_{m,1} + n_2 V_{m,2} + \ldots.. + n_i V_{m,i} + \ldots.}, \tag{4}$$

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

$$m_i = \frac{n_i}{n_{\text{solvent}} M_{\text{solvent}}} \quad \text{SI base units: mol kg}^{-1}, \tag{5}$$

where M_{solvent} is the molar mass of the solvent.

1.3. Procedures used in critical evaluation of published solubility data

Procedures used in the critical evaluation of published solubility data for crystalline nonelectrolytes dissolved in organic monosolvents and organic solvent mixtures are dependent to a large extent on the quantity and type of data to be evaluated. In those instances where independent experimental measurements exist, one can compute the mean value and standard deviation for each set of replicate values (or set of values) differ from the rest. This type of analysis will be limited primarily to the neat mono-solvents, as published data for binary and ternary solvent mixtures are relatively scarce compared to solubility data for solutes dissolved in single-solvent systems. Given the scarcity of binary solvent and ternary solvent solubility data, researchers have tended to perform measurements on new mixtures as opposed to repeating measurements on already studied mixtures, even if measured at different temperatures.

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[4]

$$-\ln x_1^{\text{ideal soly}} = \frac{\Delta H_1^{\text{fus}}}{RT}\left[1 - \frac{T}{T_{\text{mp}}}\right] + \frac{\Delta C_{p,1}}{R}\left(\frac{T_{\text{mp}} - T}{T}\right) + \frac{\Delta C_{p,1}}{R}\ln\left(\frac{T_{\text{mp}}}{T}\right), \tag{6}$$

where ΔH_1^{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. (6) can be rearranged to give

$$\ln x_1^{\text{ideal soly}} = \left[\frac{\Delta H_1^{\text{fus}}}{R T_{\text{mp}}} + \frac{\Delta C_{p,1}}{R}(1 + \ln T_{\text{mp}})\right] - \left(\frac{\Delta H_1^{\text{fus}}}{R} + \frac{\Delta C_{p,1} T_{\text{mp}}}{R}\right)\frac{1}{T} + \frac{\Delta C_{p,1}}{R}\ln T, \tag{7}$$

which has the generalized mathematical form of:

$$\ln x_1 = A + \frac{B}{T} + C \ln T. \tag{8}$$

Though derived for an ideal solution, Eq. (8) 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 published literature.

The λh model, developed by Buchowski *et al.*,[5,6] is

$$\ln\left[1 + \frac{\lambda(1 - x_1)}{x_1}\right] = \lambda h\left(\frac{1}{T} - \frac{1}{T_{\text{mp}}}\right), \tag{9}$$

a second popular mathematical representation for describing how the mole fraction solubility varies with solution temperature. In Eq. (9), 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_i values can be accurately described by either Eq. (8) and/or Eq. (9).

The solvent composition dependence upon solubility is generally evaluated using semi-theoretical solution models. During the past 50 years, more than 100 solution models have been developed for describing variation of solubility with solvent composition based on different assumptions regarding how molecules interact in solution. Predictive expressions derived from several of the proposed solution models have served as mathematical representations for isothermal solubility data in binary and ternary solvent mixtures, and for identifying experimental data points in need of redetermination. The Combined Nearly Ideal Binary Solvent (NIBS)/Redlich-Kister equation is[7,8]

$$\ln x_1^{\text{sat}} = x_2^{(\text{s})} \ln (x_1^{\text{sat}})_2 + x_3^{(\text{s})} \ln (x_1^{\text{sat}})_3 + x_2^{(\text{s})} x_3^{(\text{s})} \sum_{j=0}^{r} S_{23,j} (x_2^{(\text{s})} - x_3^{(\text{s})})^j, \qquad (10)$$

likely the most popular of the proposed mathematical representations. In the above equation, $x_i^{(\text{s})}$ refers to the initial mole fraction solvent composition of component i calculated as if the solute were not present, and $(x_\text{A}^{\text{sat}})_i$ denotes the measured solute solubility in pure solvent i. The summation in the last term on the right-hand side of Eq. (10) includes as many curve-fit $S_{23,i}$ parameters as are needed to accurately describe the observed solubility data. Generally, no more than three parameters will be needed in a given mathematical representation. The various $S_{23,i}$ parameters are determined by regression analysis.

The popularity of the Combined NIBS/Redlich-Kister model results from the fact that the computed $S_{IJ,i}$ parameters can be used to predict solute solubility in ternary solvent systems

$$\begin{aligned}\ln x_1^{\text{sat}} = {} & x_2^{(\text{s})} \ln (x_1^{\text{sat}})_2 + x_3^{(\text{s})} \ln (x_1^{\text{sat}})_3 \\ & + x_4^{(\text{s})} \ln (x_1^{\text{sat}})_4 \\ & + x_2^{(\text{s})} x_3^{(\text{s})} \sum_{j=0}^{r} S_{23,j} (x_2^{(\text{s})} - x_3^{(\text{s})})^j \\ & + x_2^{(\text{s})} x_4^{(\text{s})} \sum_{k=0}^{s} S_{24,k} (x_2^{(\text{s})} - x_4^{(\text{s})})^k \\ & + x_3^{(\text{s})} x_4^{(\text{s})} \sum_{l=0}^{t} S_{34,l} (x_3^{(\text{s})} - x_4^{(\text{s})})^l \end{aligned} \qquad (11)$$

and in higher order multicomponent solvent systems

$$\ln x_1^{\text{sat}} = \sum_{I}^{\text{Solvents}} \sum_{J>I}^{\text{Solvents}} \left[x_I^{(\text{s})} x_J^{(\text{s})} \sum_{k=0}^{n} S_{IJ,i} (x_I^{(\text{s})} - x_J^{(\text{s})})^k \right]. \qquad (12)$$

Equation (11) is referred to as the Combined Nearly Ideal Ternary Solvent (NITS)/Redlich-Kister model. To date, Eq. (11) has been shown to provide very accurate predictions for the solubility of anthracene and/or pyrene in 114 different ternary solvent mixtures including several alcohol + hydrocarbon + hydrocarbon, alcohol + alcohol + hydrocarbon, alkoxyalcohol + alcohol + hydrocarbon, alkoxyalcohol + alcohol + alcohol, and alkyl ether + alcohol + hydrocarbon solvent systems.[8–34] Predictive applicability of Eq. (11) will be illustrated in Part 2 of the planned three-part series that will update the solubilities of PAH and PAHaC in ternary organic solvent systems.

The Modified Wilson equation was used in the early to mid-1990s to mathematically describe isothermal solubility data of crystalline nonelectrolyte solutes dissolved in the binary solvent mixtures. The mathematical form of the equation is[7,8]

$$\ln (x_1^{\text{ideal soly}}/x_1) = 1 - \frac{x_2^{(\text{s})}\{1 - \ln [x_1^{\text{ideal soly}}/(x_1)_2]\}}{x_2^{(\text{s})} + x_3^{(\text{s})}\Lambda_{23}} - \frac{x_3^{(\text{s})}\{1 - \ln [x_1^{\text{ideal soly}}/(x_1)_3]\}}{x_2^{(\text{s})}\Lambda_{32} + x_3^{(\text{s})}}, \qquad (13)$$

which is considerably more complex, making the calculation of the two curve-fit parameters (Λ_{23} and Λ_{32}) more difficult. While Eq. (13) was found to accurately describe measured anthracene, carbazole, and pyrene solubility data in many different binary solvent mixtures, its use as a mathematical representation significantly decreased when the Combined NIBS/Redlich-Kister equation was extended to include ternary and higher order multicomponent solvent systems. As noted above, the curve-fit $S_{IJ,i}$ parameters in Eq. (10) can be used to estimate the solubility of crystalline solutes in ternary and higher order multicomponent solvent systems. Experimental isothermal solubility data are considered to be internally consistent if the measured x_i values can be accurately described by either Eq. (10) and/or Eq. (13).

2. Solubility of Anthracene in Binary Alkane + Alcohol Solvent Mixtures

2.1. Critical evaluation of experimental solubility data

Volume 58 in the IUPAC Solubility Data Series[2] contained solubility data for anthracene in 49 binary solvent mixtures containing hexane, heptane, octane, cyclohexane, methylcyclohexane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane (also called (1,1-dimethylethyl)cyclohexane) with 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 3-methyl-1-butanol, and 1-octanol. For the most part, the solubility data were measured at 298.2 K and seven compositions spanning the entire binary mole fraction range. To conserve space, data from the earlier volumes will not be repeated in this volume. Attention will be focused on compiling experimental values determined after Vol. 58 was published.

Acree and co-workers[35–38] determined the solubility of anthracene in binary alkane + ethanol, alkane + 1-pentanol, alkane + 2-pentanol, alkane + 2-methyl-2-propanol, alkane + 2-methyl-2-butanol, and alkane + 2-ethyl-1-hexanol at 298.15 K. The alkane solvents included hexane, heptane, octane, cyclohexane, methylcyclohexane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane. Except for the ethanol + 2,2,4-trimethylpentane solvent system, there has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. In the absence of replicate independent measurements, the experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 20 binary alkane + primary solvent systems studied are summarized in Table 1, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 1 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 2.9%, indicating that the

TABLE 1. Mathematical representation of anthracene solubilities in binary alkane (2) + alcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Hexane (2) + ethanol (3)	1.430 −0.686 1.088	0.7
Heptane (2) + ethanol (3)	1.403 −0.670 1.381	0.9
Octane (2) + ethanol (3)	1.614 −0.897 1.204	0.5
Cyclohexane (2) + ethanol (3)	1.809 −0.388 0.426	0.3
Methylcyclohexane (2) + ethanol (3)	1.898 −0.569 0.478	0.4
2,2,4-Trimethylpentane (2) + ethanol (3)	1.155[c] −0.508 1.425	0.4
2,2,4-Trimethylpentane (2) + ethanol (3)	1.096[d] −0.261 2.663	2.9
2,2,4-Trimethylpentane (2) + ethanol (3)	1.271[e] −0.407 1.702	1.5
2,2,4-Trimethylpentane (2) + ethanol (3)	1.206[f] −0.141 1.321	0.8
Octane (2) + 1-pentanol (3)	0.688 0.130 −0.241	0.7
Cyclohexane (2) + 1-pentanol (3)	0.591 0.472 0.010	0.7
Methylcyclohexane (2) + 1-pentanol (3)	0.622 0.524 0.058	0.9
2,2,4-Trimethylpentane (2) + 1-pentanol (3)	0.530 0.242 −0.011	0.5
Hexane (2) + 2-ethyl-1-hexanol (3)	0.527 0.344 0.417	0.8
Heptane (2) + 2-ethyl-1-hexanol (3)	0.389 0.166 0.131	0.2
Octane (2) + 2-ethyl-1-hexanol (3)	0.430 0.023 0.356	0.3
Cyclohexane (2) + 2-ethyl-1-hexanol (3)	0.278 0.323 0.810	0.8
Methylcyclohexane (2) + 2-ethyl-1-hexanol (3)	0.327 0.458 0.944	1.1
2,2,4-Trimethylpentane (2) + 2-ethyl-1-hexanol (3)	0.394 0.118 0.233	0.3
Heptane (2) + 2-methyl-2-propanol (3)	1.326 −0.547 0.702	0.3
Cyclohexane (2) + 2-methyl-2-propanol (3)	1.189 −0.118 0.554	0.7
Methylcyclohexane (2) + 2-methyl-2-propanol (3)	1.373 −0.165 0.369	0.5
2,2,4-Trimethylpentane (2) + 2-methyl-2-propanol (3)	1.003 −0.411 0.379	0.3

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

[c] Solubility data reported by Grubbs *et al.* at 298.15 K.

[d] Solubility data reported by Shayanfar *et al.* at 298.2 K.

[e] Solubility data reported by Shayanfar *et al.* at 308.2 K.

[f] Solubility data reported by Shayanfar *et al.* at 318.2 K.

measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The solubility of anthracene in binary 2,2,4-trimethylpentane + ethanol solvent mixtures has been measured by two research groups. Grubbs *et al.*[35] reported the solubility of anthracene in 2,2,4-trimethylpentane + ethanol mixtures at 298.2 K, while Shayanfar *et al.*[39] performed measurements at 298.2, 308.2, and 318.2 K. It is hard to compare the experimental values directly as the two sets of mole fraction solubilities in 2,2,4-trimethylpentane and ethanol differed by 9.5% and 8.9% relative percent, with the values determined by Shayanfar *et al.* being consistently larger. Differences in chemical purities and experimental methodology can lead to slight differences in values reported by independent research groups. A difference of 10% does not seem unreasonable given the differences in initial anthracene purities (99% versus 96%), and the fact that the densities of the saturated solutions were needed to convert the Shayanfar *et al.* molar solubility data to mole fraction solubilities. Any errors and/or uncertainties in the solution densities would affect the calculated mole fraction solubility. It is further noted that the solubility data of Shayanfar *et al.*[39] did exhibit the larger deviations between the observed data and back-calculated values based on Eq. (10).

The experimental anthracene solubility data are ordered according to alcohol type. Solubility data for alkane + primary alcohol solvent mixtures, for alkane + secondary solvent mixtures, and for alkane + tertiary alcohol solvent mixtures are below.

2.2. Anthracene solubility data in binary alkane + primary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) Ethanol; C_2H_6O; [64-17-5]	[35] L. M. Grubbs, K. Holley, S. S. Achi, R. Pointer, D. Casares, R. Hall, J. Ruiz, and W. E. Acree, Jr., Phys. Chem. Liq. **49**, 379 (2011).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + ethanol mixtures[a]

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000460
0.0487	0.0487	0.000555
0.0967	0.0966	0.000641
0.2286	0.2284	0.000840
0.3049	0.3046	0.000923
0.4053	0.4049	0.001028
0.6434	0.6426	0.001220
0.7786	0.7776	0.001281
1.0000	0.9987	0.001274

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, Aldrich Chemical Company.
(3) 99%, Aaper Alcohol and Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-85-5] (3) Ethanol; C_2H_6O; [64-17-5]	[35]L. M. Grubbs, K. Holley, S. S. Achi, R. Pointer, D. Casares, R. Hall, J. Ruiz, and W. E. Acree, Jr., Phys. Chem. Liq. **49**, 379 (2011).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + ethanol mixtures[a]

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000460
0.0454	0.0454	0.000561
0.0968	0.0956	0.000661
0.2124	0.2122	0.000869
0.2872	0.2869	0.000976
0.3837	0.3833	0.001105
0.5980	0.5972	0.001336
0.7425	0.7414	0.001484
1.0000	0.9984	0.001571

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99%, anhydrous, Aldrich Chemical Company.
(3) 99%, Aaper Alcohol and Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) Ethanol; C_2H_6O; [64-17-5]	[35]L. M. Grubbs, K. Holley, S. S. Achi, R. Pointer, D. Casares, R. Hall, J. Ruiz, and W. E. Acree, Jr., Phys. Chem. Liq. **49**, 379 (2011).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + ethanol mixtures[a]

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000460
0.0445	0.0445	0.000566
0.0843	0.0842	0.000661
0.1966	0.1964	0.000919
0.2653	0.2650	0.001032
0.3544	0.3540	0.001176
0.6015	0.6006	0.001520
0.7444	0.7431	0.001700
1.0000	0.9982	0.001838

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, Aldrich Chemical Company.
(3) 99%, Aaper Alcohol and Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Ethanol; C_2H_6O; [64-17-5]	[35]L. M. Grubbs, K. Holley, S. S. Achi, R. Pointer, D. Casares, R. Hall, J. Ruiz, and W. E. Acree, Jr., Phys. Chem. Liq. **49**, 379 (2011).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + ethanol mixtures[a]

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000460
0.0580	0.0580	0.000565
0.1121	0.1120	0.000668
0.2709	0.2706	0.000963
0.3426	0.3422	0.001099
0.4467	0.4461	0.001241
0.6777	0.6766	0.001530
0.8262	0.8249	0.001614
1.0000	0.9984	0.001553

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, HPLC grade, Aldrich Chemical Company.
(3) 99%, Aaper Alcohol and Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) Ethanol; C_2H_6O; [64-17-5]	[35]L. M. Grubbs, K. Holley, S. S. Achi, R. Pointer, D. Casares, R. Hall, J. Ruiz, and W. E. Acree, Jr., Phys. Chem. Liq. **49**, 379 (2011).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + ethanol mixtures[a]

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000460
0.0515	0.0515	0.000562
0.1080	0.1079	0.000683
0.2366	0.2364	0.000952
0.3097	0.3094	0.001092
0.4110	0.4105	0.001257
0.6559	0.6549	0.001579
0.8007	0.7993	0.001688
1.0000	0.9984	0.001649

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Aaper Alcohol and Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) Ethanol; C_2H_6O; [64-17-5]	[35]L. M. Grubbs, K. Holley, S. S. Achi, R. Pointer, D. Casares, R. Hall, J. Ruiz, and W. E. Acree, Jr., Phys. Chem. Liq. **49**, 379 (2011).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + ethanol mixtures[a]

$x_2^{(s)}$	x_2	x_1
0.0000	0.0000	0.000460
0.0437	0.0437	0.000538
0.0805	0.0805	0.000594
0.1898	0.1897	0.000737
0.2621	0.2619	0.000797
0.3329	0.3326	0.000850
0.5830	0.5824	0.000997
0.7237	0.7229	0.001078
1.0000	0.9989	0.001074

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; x_1: mole fraction solubility of the solute; x_2: mole fraction of component 2 in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99.7%, HPLC grade, Aldrich Chemical Company.
(3) 99%, Aaper Alcohol and Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) Ethanol; C_2H_6O; [64-17-5]	[39]A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).
Variables:	**Prepared by:**
T/K = 298.2, 308.2, 318.2; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + ethanol mixtures[a]

T/K	$x_3^{(s)}$	x_3	x_1
298.2	0.000	0.000	0.001187
	0.239	0.239	0.001277
	0.414	0.414	0.001143
	0.548	0.547	0.001041
	0.653	0.652	0.000950
	0.739	0.738	0.000885
	0.809	0.808	0.000821
	0.868	0.867	0.000742
	0.919	0.918	0.000673
	0.962	0.961	0.000608
	1.000	0.999	0.000505
308.2	0.000	0.000	0.001515
	0.242	0.242	0.001610
	0.418	0.417	0.001466
	0.552	0.551	0.001359
	0.657	0.656	0.001244
	0.742	0.741	0.001160
	0.812	0.811	0.001059
	0.870	0.869	0.000959
	0.920	0.919	0.000862
	0.963	0.962	0.000777
	1.000	0.999	0.000665
318.2	0.000	0.000	0.001768
	0.240	0.240	0.001898
	0.415	0.414	0.001705
	0.549	0.548	0.001548
	0.654	0.653	0.001404
	0.739	0.738	0.001295
	0.810	0.809	0.001214
	0.869	0.868	0.001087
	0.919	0.918	0.000979
	0.962	0.961	0.000884
	1.000	0.999	0.000780

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

Auxiliary Information

Method/Apparatus/Procedure:

Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.9%, Merck Chemical Company, Germany, no further purification specified.

Estimated Error:

Temperature: ±0.2 K.
$x_3^{(s)}$: ±0.001.
x_1: ±2.7% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[36]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., P. H. Flanders, V. G. Varanasi, and S. W. Campbell, Fluid Phase Equilib. **134**, 185 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1262	0.1260	0.001351
0.2341	0.2338	0.001377
0.4343	0.4337	0.001368
0.5444	0.5437	0.001336
0.6461	0.6453	0.001284
0.8353	0.8343	0.001189
0.9095	0.9085	0.001145
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-85-5] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[36]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., P. H. Flanders, V. G. Varanasi, and S. W. Campbell, Fluid Phase Equilib. **134**, 185 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1405	0.1403	0.001622
0.2547	0.2543	0.001627
0.4681	0.4674	0.001551
0.5639	0.5631	0.001490
0.6745	0.6736	0.001402
0.8242	0.8232	0.001271
0.9160	0.9150	0.001180
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1484	0.1481	0.001859
0.2791	0.2786	0.001816
0.5026	0.5018	0.001668
0.6018	0.6009	0.001572
0.6974	0.6964	0.001476
0.8595	0.8584	0.001256
0.9270	0.9259	0.001166
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ± 0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.0946	0.0944	0.001643
0.2023	0.2020	0.001646
0.4103	0.4097	0.001578
0.5108	0.5100	0.001501
0.6088	0.6079	0.001427
0.7975	0.7965	0.001248
0.8991	0.9988	0.001154
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ± 0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-97-2] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1269	0.1267	0.001778
0.2316	0.2312	0.001734
0.4458	0.4451	0.001615
0.5347	0.5339	0.001542
0.6304	0.6295	0.001451
0.8161	0.8151	0.001245
0.9074	0.9064	0.001157
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1428	0.1426	0.001182
0.2960	0.2956	0.001224
0.5244	0.5238	0.001235
0.6141	0.6134	0.001214
0.7171	0.7162	0.001196
0.8440	0.8430	0.001143
0.9318	0.9308	0.001115
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.0983	0.0982	0.001422
0.1794	0.1791	0.001469
0.3597	0.3592	0.001516
0.4565	0.4559	0.001525
0.5590	0.5581	0.001529
0.7647	0.7635	0.001504
0.8718	0.9705	0.001451
1.0000	0.9986	0.001397

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Heptane; C_7H_{16}; [142-82-5]
(3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

Original Measurements:
[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1116	0.1114	0.001647
0.1972	0.1969	0.001669
0.3931	0.3924	0.001656
0.4806	0.4798	0.001639
0.5718	0.5709	0.001615
0.7850	0.7838	0.001517
0.8865	0.8852	0.001464
1.0000	0.9986	0.001397

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Octane; C_8H_{18}; [111-65-9]
(3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

Original Measurements:
[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1190	0.1188	0.001907
0.2139	0.2135	0.001898
0.4149	0.4141	0.001835
0.5098	0.5089	0.001785
0.6148	0.6137	0.001712
0.8102	0.8089	0.001606
0.8932	0.8918	0.001527
1.0000	0.9986	0.001397

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

Original Measurements:
[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.0590	0.0589	0.001658
0.1441	0.1439	0.001689
0.3159	0.3154	0.001659
0.4036	0.4029	0.001632
0.5098	0.5090	0.001596
0.7412	0.7401	0.001535
0.8616	0.8603	0.001492
1.0000	0.9986	0.001397

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]
(3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

Original Measurements:

[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.0890	0.0888	0.001830
0.1771	0.1768	0.001819
0.3610	0.3604	0.001726
0.4509	0.4501	0.001685
0.5499	0.5490	0.001633
0.7667	0.7655	0.001563
0.8751	0.8736	0.001498
1.0000	0.9986	0.001397

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

Original Measurements:

[37]L. E. Roy, C. E. Hernández, G. D. Reddy, J. T. Sanders, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., J. Chem. Eng. Data **43**, 493 (1998).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1144	0.1143	0.001184
0.2135	0.2132	0.001232
0.4193	0.4187	0.001325
0.5143	0.5136	0.001357
0.6103	0.6095	0.001387
0.7935	0.7924	0.001415
0.8027	0.8016	0.001419
0.8974	0.8961	0.001414
1.0000	0.9986	0.001397

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

2.3. Anthracene solubility data in binary alkane + secondary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-85-5] (3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[36]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., P. H. Flanders, V. G. Varanasi, and S. W. Campbell, Fluid Phase Equilib. **134**, 185 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1469	0.1467	0.001578
0.2544	0.2540	0.001547
0.4611	0.4604	0.001427
0.5702	0.5694	0.001333
0.6693	0.6685	0.001244
0.8386	0.8377	0.001030
0.9198	0.9190	0.000916
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

2.4. Anthracene solubility data in binary alkane + tertiary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Methyl-2-propanol; $C_4H_{10}O$; [64-17-5]	[38]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-methyl-2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1354	0.1352	0.001536
0.2898	0.2894	0.001382
0.5134	0.5128	0.001137
0.5993	0.5987	0.001025
0.7060	0.7054	0.000892
0.8485	0.8479	0.000677
0.9172	0.9168	0.000570
1.0000	0.9996	0.000430

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Methyl-2-propanol; $C_4H_{10}O$; [64-17-5]	[38]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-methyl-2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1213	0.1211	0.001553
0.2219	0.2216	0.001446
0.4242	0.4237	0.001187
0.5264	0.5258	0.001074
0.6314	0.6308	0.000933
0.8199	0.8193	0.000677
0.9072	0.9067	0.000555
1.0000	0.9996	0.000430

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Methyl-2-propanol; $C_4H_{10}O$; [64-17-5]	[38]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-methyl-2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1382	0.1380	0.001632
0.2612	0.2608	0.001506
0.4844	0.4838	0.001200
0.5682	0.5676	0.001086
0.6681	0.6675	0.000940
0.8386	0.8380	0.000669
0.9143	0.9138	0.000553
1.0000	0.9996	0.000430

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(3) 2-Methyl-2-propanol; $C_4H_{10}O$; [64-17-5]

Original Measurements:

[38]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; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-methyl-2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1655	0.1653	0.001049
0.3092	0.3089	0.000972
0.5406	0.5401	0.000847
0.6368	0.6363	0.000781
0.6887	0.6882	0.000747
0.8761	0.8756	0.000569
0.9321	0.9316	0.000507
1.0000	0.9996	0.000430

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Heptane; C_7H_{16}; [142-85-5]
(3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]

Original Measurements:

[36]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., P. H. Flanders, V. G. Varanasi, and S. W. Campbell, Fluid Phase Equilib. **134**, 185 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1483	0.1481	0.001543
0.2563	0.2559	0.001493
0.4661	0.4655	0.001326
0.5728	0.5721	0.001237
0.6721	0.6713	0.001149
0.8491	0.8483	0.000980
0.9281	0.9273	0.000884
1.0000	0.9992	0.000790

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

3. Solubility of Anthracene in Binary Alkane + Chloroalkane Solvent Mixtures

3.1. Critical evaluation of experimental solubility data

Volume 54 in the IUPAC Solubility Data Series[1] contained solubility data for anthracene in 16 binary solvent mixtures containing tetrachloromethane, 1-chlorobutane, and 1,4-dichlorobutane with hexane, heptane, octane, cyclohexane, methylcyclohexane, and 2,2,4-trimethylpentane. The experimental data were measured at 298.15 K. To conserve space, data from the earlier volume will not repeated here.

Acree and co-workers[40] have reported the solubility of anthracene in binary alkane + 1-chlorooctane and alkane + chlorocyclohexane solvent mixtures at 298.2 K. The alkane cosolvents include hexane, heptane, octane, cyclohexane, methylcyclohexane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane (also called (1,1-dimethylethyl)cyclohexane). There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. In the absence of replicate independent measurements, the experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 14 binary alkane + chloroalkane solvent systems studied are summarized in Table 2, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 2 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.3% to 0.8%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

TABLE 2. Mathematical representation of anthracene solubilities in binary alkane (2) + chloroalkane (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Hexane (2) + 1-chlorooctane (3)	1.287	0.3
	0.397	
Heptane (2) + 1-chlorooctane (3)	0.918	0.8
Octane (2) + 1-chlorooctane (3)	0.618	0.7
Cyclohexane (2) + 1-chlorooctane (3)	1.265	0.6
	0.657	
	0.320	
Methylcyclohexane (2) + 1-chlorooctane (3)	1.034	0.7
	0.533	
	0.446	
2,2,4-Trimethylpentane (2) + 1-chlorooctane (3)	1.065	0.5
	0.083	
	0.220	
tert-Butylcyclohexane (2) + 1-chlorooctane	0.721	0.2
	0.165	
Hexane (2) + chlorocyclohexane (3)	1.098	0.6
	0.209	
	0.085	
Heptane (2) + chlorocyclohexane (3)	0.796	0.4
Octane (2) + chlorocyclohexane (3)	0.571	0.8
Cyclohexane (2) + chlorocyclohexane (3)	0.940	0.3
	0.346	
	0.119	
Methylcyclohexane (2) + chlorocyclohexane (3)	0.841	0.8
	0.327	
	0.353	
2,2,4-Trimethylpentane (2) + chlorocyclohexane (3)	0.626	0.2
	0.146	
	−0.133	
tert-Butylcyclohexane (2) + chlorocyclohexane (3)	0.402	0.5
	0.075	
	−0.263	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only a single coefficient is listed, then $S_{23,1}$ and $S_{23,2}$ are zero. Similarly, if two coefficients are listed, then $S_{23,2}$ is zero.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

The experimental anthracene solubility data for binary alkane + 1-chlorooctane solvent mixtures and binary alkane + chlorocyclohexane solvent mixtures are given in Secs. 3.2 and 3.3.

3.2. Anthracene solubility data in binary alkane + 1-chlorooctane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40] C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.0909	0.0907	0.001718
0.1663	0.1659	0.002130
0.3360	0.3349	0.003217
0.4170	0.4154	0.003773
0.5365	0.5340	0.004579
0.7350	0.7306	0.005924
0.8715	0.8655	0.006918
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.0921	0.0918	0.001972
0.1797	0.1793	0.002419
0.3626	0.3613	0.003518
0.4635	0.4616	0.004152
0.5606	0.5579	0.004767
0.7790	0.7740	0.006315
0.8782	0.8720	0.007036
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.0999	0.0997	0.002238
0.1944	0.1939	0.002673
0.3811	0.3797	0.003728
0.4837	0.4816	0.004354
0.5938	0.5912	0.004974
0.7855	0.7806	0.006289
0.8862	0.8799	0.007061
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.0712	0.0711	0.002000
0.1381	0.1378	0.002427
0.3005	0.2994	0.003516
0.3771	0.3756	0.004001
0.4928	0.4905	0.004676
0.7109	0.7065	0.006161
0.8321	0.8265	0.006751
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.0814	0.0812	0.002152
0.1521	0.1517	0.002556
0.3321	0.3309	0.003642
0.4287	0.4269	0.004192
0.5373	0.5346	0.004936
0.7485	0.7438	0.006219
0.8662	0.8602	0.006973
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1078	0.1076	0.001498
0.1980	0.1976	0.001929
0.3939	0.3927	0.003073
0.4958	0.4940	0.003728
0.5981	0.5954	0.004474
0.7796	0.7749	0.006085
0.8966	0.8903	0.007045
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + 1-chlorooctane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1053	0.1050	0.002479
0.2018	0.2012	0.002967
0.4072	0.4055	0.004138
0.4938	0.4915	0.004662
0.6093	0.6060	0.005389
0.7690	0.7640	0.006524
0.8900	0.8837	0.007081
1.0000	0.9922	0.007780

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

3.3. Anthracene solubility data in binary alkane + chlorocyclohexane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1112	0.1110	0.001735
0.2203	0.2198	0.002236
0.4256	0.4242	0.003355
0.5154	0.5134	0.003809
0.6173	0.6146	0.004402
0.8145	0.8101	0.005450
0.8078	0.8030	0.005919
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1331	0.1328	0.002072
0.2419	0.2413	0.002543
0.4466	0.4450	0.003550
0.5560	0.5537	0.004197
0.6565	0.6534	0.004688
0.8369	0.8322	0.005656
0.9205	0.9150	0.005995
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1498	0.1494	0.002373
0.2540	0.2533	0.002825
0.5037	0.5017	0.003889
0.5822	0.5797	0.004330
0.6759	0.6726	0.004881
0.8457	0.8409	0.005697
0.9223	0.9168	0.005993
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]

Original Measurements:

[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1044	0.1042	0.002029
0.1966	0.1061	0.002475
0.3658	0.3646	0.003320
0.4713	0.4695	0.003803
0.5864	0.5838	0.004413
0.7843	0.7801	0.005355
0.8797	0.8746	0.005800
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]
(3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]

Original Measurements:

[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1083	0.1081	0.002175
0.2219	0.2213	0.002675
0.4146	0.4131	0.003582
0.5062	0.5041	0.004060
0.6302	0.6273	0.004673
0.8082	0.8038	0.005465
0.8832	0.8780	0.005915
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [548-84-1] (3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1416	0.1414	0.001499
0.2708	0.2703	0.001974
0.4788	0.4774	0.002951
0.5672	0.5653	0.003422
0.6562	0.6536	0.003920
0.8554	0.8510	0.005185
0.9287	0.9234	0.005753
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]	[40]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, M. E. R. McHale, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 954 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + chlorocyclohexane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1530	0.1526	0.002471
0.2741	0.2733	0.002930
0.5020	0.5000	0.003899
0.5898	0.5872	0.004373
0.6916	0.6883	0.004738
0.8522	0.8475	0.005506
0.9252	0.9198	0.005878
1.0000	0.9936	0.006353

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

4. Solubility of Anthracene in Binary Alkane + Ether Solvent Mixtures

4.1. Critical evaluation of experimental solubility data

Volume 54 in the IUPAC Solubility Data Series[1] contained solubility data for anthracene in 22 binary solvent mixtures containing 1,1′-oxybisbutane, 1,4-dioxane, and tetrahydropyran with hexane, heptane, octane, hexadecane, cyclohexane, methylcyclohexane, cyclooctane, 2,2,4-trimethylpentane, and squalane. The experimental data were measured at 298.15 K. To conserve space, data from the earlier volume will not repeated here.

Acree and co-workers[41–43] determined the solubility of anthracene in several binary solvent mixtures containing

2,2′-oxybispropane, 2-methoxy-2-methylpropane (also called methyl *tert*-butyl ether) and 1,1′-oxybis[2-methoxyethane] with hexane, heptane, octane, cyclohexane, methylcyclohexane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane (also called (1,1-dimethylethyl)cyclohexane) at 298.15 K. There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 19 binary alkane + ether systems studied are summarized in Table 3, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 3 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 0.8%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental anthracene solubility data are given in Secs. 4.2–4.4 for binary alkane + 2,2′-oxybispropane solvent mixtures, for binary alkane + 2-methoxy-2-methylpropane solvent mixtures, and for binary alkane + 1,1′-oxybis[2-methoxyethane] solvent mixtures.

TABLE 3. Mathematical representation of anthracene solubilities in binary alkane (2) + ether (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Hexane (2) + 2,2′-oxybispropane (3)	0.195 0.177 0.490	0.3
Heptane (2) + 2,2′-oxybispropane (3)	0.153	0.2
Octane (2) + 2,2′-oxybispropane (3)	0.216 −0.084 0.258	0.3
Cyclohexane (2) + 2,2′-oxybispropane (3)	0.546 0.303 0.205	0.3
Methylcyclohexane (2) + 2,2′-oxybispropane (3)	0.494 0.219 0.325	0.4
2,2,4-Trimethylpentane (2) + 2,2′-oxybispropane (3)	0.113 −0.036 0.177	0.4
Hexane (2) + 2-methoxy-2-methylpropane (3)	0.318 −0.244	0.2
Heptane (2) + 2-methoxy-2-methylpropane (3)	0.149 −0.268	0.5
Octane (2) + 2-methoxy-2-methylpropane (3)	0.116 −0.203 0.098	0.2
Cyclohexane (2) + 2-methoxy-2-methylpropane (3)	0.741 0.174 −0.305	0.7
Methylcyclohexane (2) + 2-methoxy-2-methylpropane (3)	0.638	0.2
2,2,4-Trimethylpentane (2) + 2-methoxy-2-methylpropane (3)	−0.072 −0.294	0.5
tert-Butylcyclohexane + 2-methoxy-2-methylpropane (3)	−0.126 −0.197	0.4
Hexane (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.268 0.641 0.159	0.7
Heptane (2) + 1,1′-oxybis[2-methoxyethane] (3)	1.869 0.437 0.233	0.2
Octane (2) + 1,1′-oxybis[2-methoxyethane] (3)	1.616 0.256 0.320	0.4
Cyclohexane (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.475 1.267 0.825	0.5
Methylcyclohexane (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.210 1.068 0.667	0.8
2,2,4-Trimethylpentane (2) + 1,1′-oxybis[2-methoxyethane] (3)	1.953 0.440 0.178	0.2

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only a single coefficient is listed, then $S_{23,1}$ and $S_{23,2}$ are zero. Similarly, if two coefficients are listed, then $S_{23,2}$ is zero.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

4.2. Anthracene solubility data in binary alkane + 2,2′-oxybispropane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[41] M. Carrillo, M. Corella, K. Wolcott, K. R. Bowen, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 270 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1098	0.1096	0.001463
0.2022	0.2019	0.001570
0.3817	0.3810	0.001756
0.4835	0.4826	0.001877
0.5841	0.5821	0.001980
0.7732	0.7715	0.002238
0.8892	0.8870	0.002419
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[41]M. Carrillo, M. Corella, K. Wolcott, K. R. Bowen, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 270 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001576
0.1357	0.1355	0.001711
0.2247	0.2243	0.001799
0.4129	0.4121	0.001981
0.5041	0.5031	0.002074
0.6102	0.6089	0.002180
0.7970	0.7951	0.002337
0.8930	0.8908	0.002430
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[41]M. Carrillo, M. Corella, K. Wolcott, K. R. Bowen, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 270 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1401	0.1398	0.001991
0.2374	0.2369	0.002064
0.4358	0.4348	0.002202
0.5378	0.5366	0.002311
0.6317	0.6302	0.002383
0.8188	0.8167	0.002504
0.8840	0.8818	0.002533
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]

Original Measurements:
[41]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1004	0.1002	0.001768
0.1502	0.1499	0.001867
0.3444	0.3437	0.002145
0.4344	0.4334	0.002202
0.4356	0.4346	0.002213
0.5831	0.5818	0.002313
0.7577	0.7559	0.002435
0.8688	0.8666	0.002480
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99.9+%, HPLC grade, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Methylcyclohexane; C_7H_{14}; [110-54-3]
(3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]

Original Measurements:
[41]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.0990	0.0988	0.001860
0.1945	0.1941	0.002020
0.2898	0.2892	0.002121
0.3721	0.3713	0.002182
0.4754	0.4743	0.002296
0.7632	0.7610	0.002946
0.8924	0.8902	0.002520
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]

Original Measurements:
[41]M. Carrillo, M. Corella, K. Wolcott, K. R. Bowen, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 270 (2007).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1349	0.1347	0.001229
0.2408	0.2405	0.001356
0.4530	0.4523	0.001627
0.5410	0.5401	0.001752
0.6343	0.6331	0.001897
0.8184	0.8166	0.002219
0.9086	0.9064	0.002380
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99.7%, HPLC grade, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

4.3. Anthracene solubility data in binary alkane + 2-methoxy-2-methylpropane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00127
0.1216	0.1214	0.00144
0.2175	0.2172	0.00159
0.4207	0.4199	0.00197
0.5240	0.5229	0.00218
0.6328	0.6313	0.00242
0.7979	0.7958	0.00274
0.9058	0.9031	0.00294
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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+%, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00157
0.1425	0.1423	0.00171
0.2263	0.2259	0.00184
0.4551	0.4541	0.00219
0.5581	0.5568	0.00237
0.6492	0.6475	0.00255
0.8292	0.8268	0.00284
0.9098	0.9071	0.00297
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00184
0.1376	0.1373	0.00198
0.2592	0.2587	0.00211
0.4711	0.4700	0.00239
0.5759	0.5744	0.00255
0.6774	0.6756	0.00272
0.8451	0.8426	0.00292
0.9173	0.9145	0.00301
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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+%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00155
0.0935	0.0933	0.00174
0.1765	0.1762	0.00195
0.3737	0.3728	0.00242
0.4779	0.4767	0.00258
0.5822	0.5806	0.00268
0.7800	0.7777	0.00289
0.9079	0.9052	0.00295
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00165
0.1120	0.1118	0.00189
0.2070	0.2066	0.00208
0.4072	0.4062	0.00245
0.5135	0.5121	0.00265
0.5953	0.5937	0.00277
0.7875	0.7852	0.00298
0.9008	0.8981	0.00303
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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+%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00107
0.1411	0.1409	0.00120
0.2681	0.2677	0.00138
0.4838	0.4830	0.00175
0.5787	0.5776	0.00194
0.6793	0.6778	0.00217
0.8453	0.8431	0.00264
0.9408	0.9381	0.00291
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[42]M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 1203 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00198
0.1560	0.1557	0.00219
0.2707	0.2643	0.00237
0.4880	0.4867	0.00272
0.5887	0.5870	0.00285
0.6928	0.6907	0.00297
0.8487	0.8461	0.00301
0.9207	0.9179	0.00304
1.0000	0.9969	0.00305

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

4.4. Anthracene solubility data in binary alkane + 1,1′-oxybis[2-methoxyethane] solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[43]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00127
0.1091	0.1089	0.00212
0.1841	0.1836	0.00289
0.3538	0.3521	0.00493
0.4792	0.4761	0.00639
0.5568	0.5527	0.00734
0.7909	0.7831	0.00991
0.8892	0.8796	0.01076
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[43]K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00157
0.1128	0.1125	0.00248
0.2099	0.2092	0.00334
0.4080	0.4057	0.00566
0.4810	0.4779	0.00648
0.6097	0.6048	0.00806
0.8073	0.7991	0.01012
0.8872	0.8777	0.01075
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized three times from acetone.

(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.

(3) 99.5%, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[43]K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00184
0.1244	0.1240	0.00286
0.2342	0.2252	0.00384
0.4310	0.4284	0.00608
0.5319	0.5280	0.00728
0.6076	0.6027	0.00800
0.8240	0.8164	0.01041
0.9018	0.8919	0.01099
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized three times from acetone.

(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.

(3) 99.5%, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[43]K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00155
0.0790	0.0788	0.00246
0.1688	0.1682	0.00360
0.3439	0.3418	0.00598
0.4251	0.4221	0.00698
0.5395	0.5351	0.00820
0.7485	0.7408	0.01027
0.8734	0.8638	0.01097
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[43]K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00165
0.1096	0.1093	0.00287
0.1942	0.1934	0.00388
0.3784	0.3761	0.00610
0.4726	0.4592	0.00726
0.5848	0.5798	0.00847
0.7786	0.7706	0.01027
0.8821	0.8725	0.01086
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[43]K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Chem. Eng. Commun. **162**, 215 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00107
0.1162	0.1160	0.00180
0.2181	0.2175	0.00264
0.4370	0.4348	0.00492
0.5321	0.5289	0.00609
0.6354	0.6307	0.00736
0.7899	0.7826	0.00930
0.9025	0.8930	0.01051
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized three times from acetone.

(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.

(3) 99.5%, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

5. Solubility of Anthracene in Binary Alkane + Alkoxyalcohol Solvent Mixtures

5.1. Critical evaluation of experimental solubility data

Acree and co-workers[44–48] determined the solubility of anthracene in several binary alkane + 2-ethoxyethanol, alkane + 2-propoxyethanol, alkane + 2-isopropoxyethanol, alkane + 2-butoxyethanol, and alkane + 3-methoxy-1-butanol solvent mixtures at 298.15 K. The alkane cosolvents include hexane, heptane, octane, cyclohexane, methylcyclohexane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane (also called (1,1-dimethylethyl)cyclohexane). There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 34 binary alkane + alkoxyalcohol solvent systems studied are summarized in Table 4, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 4 reveals that Eq. (10) does provide a very accurate

TABLE 4. Mathematical representation of anthracene solubilities in binary alkane (2) + alkoxyalcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Hexane (2) + 2-ethoxyethanol (3)	1.434 0.126 0.526	0.6
Heptane (2) + 2-ethoxyethanol (3)	1.220 −0.168 0.594	0.2
Octane (2) + 2-ethoxyethanol (3)	1.158 −0.205 0.571	0.3
Cyclohexane (2) + 2-ethoxyethanol (3)	1.606 0.354 0.374	0.5
Methylcyclohexane (2) + 2-ethoxyethanol (3)	1.410 0.289 0.613	0.6
2,2,4-Trimethylpentane (2) + 2-ethoxyethanol (3)	1.101 −0.134 0.475	0.3
Hexane (2) + 2-propoxyethanol (3)	1.319 0.442 0.361	0.2
Heptane (2) + 2-propoxyethanol (3)	0.977 0.290 0.219	0.2
Octane (2) + 2-propoxyethanol (3)	0.994 0.091 0.209	0.2
Cyclohexane (2) + 2-propoxyethanol (3)	1.260 0.756 0.518	0.5
Methylcyclohexane (2) + 2-propoxyethanol (3)	1.214 0.634 0.531	0.8
2,2,4-Trimethylpentane (2) + 2-propoxyethanol (3)	0.978 0.234 0.343	0.2
tert-Butylcyclohexane (2) + 2-propoxyethanol (3)	1.041 0.246 0.274	0.7
Hexane (2) + 2-isopropoxyethanol (3)	1.282 0.462 0.336	0.3
Heptane (2) + 2-isopropoxyethanol (3)	1.018 0.322 0.103	0.4
Octane (2) + 2-isopropoxyethanol (3)	0.930 0.291 0.084	0.6
Cyclohexane (2) + 2-isopropoxyethanol (3)	1.297 0.755 0.216	0.5

TABLE 4. Mathematical representation of anthracene solubilities in binary alkane (2) + alkoxyalcohol (3) solvent mixtures—Continued

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Methylcyclohexane (2) + 2-isopropoxyethanol (3)	1.185 0.650 0.460	1.1
2,2,4-Trimethylpentane (2) + 2-isopropoxyethanol (3)	0.912 0.364 0.113	0.2
tert-Butylcyclohexane (2) + 2-isopropoxyethanol (3)	1.016 0.350 0.153	0.6
Hexane (2) + 2-butoxyethanol (3)	1.217 0.679 0.224	0.3
Heptane (2) + 2-butoxyethanol (3)	0.928 0.488 0.123	0.5
Octane (2) + 2-butoxyethanol (3)	0.832 0.366 0.105	0.3
Cyclohexane (2) + 2-butoxyethanol (3)	1.081 0.863 0.565	0.4
Methylcyclohexane (2) + 2-butoxyethanol (3)	0.992 0.868 0.489	0.7
2,2,4-Trimethylpentane (2) + 2-butoxyethanol (3)	0.883 0.548 0.108	0.8
tert-Butylcyclohexane (2) + 2-Butoxyethanol (3)	0.883 0.427 0.275	0.6
Hexane (2) + 3-methoxy-1-butanol (3)	1.489 0.344 0.189	0.7
Heptane (2) + 3-methoxy-1-butanol (3)	1.196 0.217 0.476	0.8
Octane (2) + 3-methoxy-1-butanol (3)	1.088 −0.032 0.516	0.4
Cyclohexane (2) + 3-methoxy-1-butanol (3)	1.480 0.670 0.465	0.6
Methylcyclohexane (2) + 3-methoxy-1-butanol (3)	1.459 0.377 0.692	1.0
2,2,4-Trimethylpentane (2) + 3-methoxy-1-butanol (3)	1.108 0.265 0.487	0.5
tert-Butylcyclohexane (2) + 3-methoxy-1-butanol (3)	1.199 0.084 0.353	0.3

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 1.1%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental solubility data for binary alkane + 2-ethoxyethanol solvent mixtures, for binary alkane + 2-propoxyethanol solvent mixtures, for binary alkane + 2-isopropoxyethanol solvent mixtures, for binary alkane + 2-butoxyethanol solvent mixtures, and for binary alkane + 3-methoxy-1-butanol solvent mixtures are given in Secs. 5.2–5.6.

5.2. Anthracene solubility data in binary alkane + 2-ethoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[44] 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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1278	0.1276	0.001740
0.2647	0.2641	0.002157
0.4837	0.4824	0.002698
0.5851	0.5834	0.002947
0.6786	0.6765	0.003106
0.8386	0.8360	0.003158
0.9340	0.9311	0.003074
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Heptane; C_7H_{16}; [142-82-5]
(3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]

Original Measurements:
[44]C. E. Hernández, L. E. Roy, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 677 (1999).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1583	0.1580	0.002085
0.2787	0.2780	0.002402
0.5044	0.5029	0.002920
0.6029	0.6010	0.003109
0.6998	0.6975	0.003229
0.8573	0.8545	0.003276
0.9265	0.9236	0.003152
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Octane; C_8H_{18}; [111-65-9]
(3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]

Original Measurements:
[44]C. E. Hernández, L. E. Roy, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 677 (1999).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1779	0.1775	0.002397
0.2987	0.2979	0.002703
0.5246	0.5229	0.003146
0.6224	0.6204	0.003278
0.7186	0.7162	0.003376
0.8679	0.8650	0.003293
0.9315	0.9285	0.003173
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]

Original Measurements:
[44]C. E. Hernández, L. E. Roy, T. Deng, M. B. Tuggle, and W. E. Acree, Jr., Phys. Chem. Liq. **37**, 677 (1999).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1151	0.1149	0.002076
0.2195	0.2190	0.002461
0.4346	0.4333	0.003051
0.5300	0.5283	0.003238
0.6247	0.6226	0.003321
0.8151	0.8124	0.003287
0.9033	0.9005	0.003142
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[44]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1224	0.1221	0.002196
0.2531	0.2524	0.002604
0.4700	0.4686	0.003059
0.5773	0.5754	0.003224
0.6745	0.6723	0.003313
0.8452	0.8424	0.003266
0.9181	0.9152	0.003134
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[44]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1778	0.1775	0.001528
0.3156	0.3150	0.001885
0.5317	0.5304	0.002420
0.6207	0.6191	0.002609
0.7288	0.7260	0.003859
0.8670	0.8644	0.003020
0.9376	0.9348	0.003013
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

5.3. Anthracene solubility data in binary alkane + 2-propoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1249	0.1247	0.001759
0.2326	0.2321	0.002146
0.4317	0.4305	0.002711
0.5320	0.5304	0.002953
0.6522	0.6502	0.003132
0.8262	0.8234	0.003357
0.9002	0.8972	0.003380
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.0978	0.0976	0.001908
0.2328	0.2323	0.002308
0.4686	0.4673	0.002874
0.5579	0.5562	0.003031
0.6638	0.6617	0.003165
0.8444	0.8416	0.003346
0.9301	0.9270	0.003357
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1508	0.1504	0.002338
0.2637	0.2630	0.002646
0.4798	0.4783	0.003140
0.5839	0.5820	0.003302
0.6912	0.6888	0.003448
0.8465	0.8435	0.003493
0.9284	0.9252	0.003435
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.0890	0.0888	0.002003
0.1777	0.1773	0.002341
0.3903	0.3891	0.002949
0.4892	0.4876	0.003127
0.5941	0.5922	0.003238
0.8009	0.7982	0.003368
0.8854	0.8824	0.003377
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1025	0.1023	0.002154
0.2075	0.2070	0.002520
0.4274	0.4261	0.003039
0.5240	0.5223	0.003233
0.6156	0.6135	0.003355
0.8149	0.8121	0.003416
0.9246	0.9214	0.003409
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1322	0.1320	0.001458
0.2477	0.2473	0.001764
0.4922	0.4910	0.002402
0.5876	0.5861	0.002631
0.6856	0.6836	0.002872
0.8605	0.8577	0.003217
0.9286	0.9255	0.003297
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[45]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1468	0.1465	0.002245
0.2793	0.2785	0.002880
0.4952	0.4936	0.003307
0.6002	0.5981	0.003457
0.6974	0.6949	0.003549
0.8544	0.8514	0.003524
0.9230	0.9198	0.003442
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

5.4. Anthracene solubility data in binary alkane + 2-isopropoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1110	0.1108	0.001686
0.2247	0.2242	0.002073
0.4685	0.4672	0.002687
0.5285	0.5270	0.002778
0.6392	0.6373	0.002950
0.8258	0.8232	0.003133
0.9068	0.9040	0.003125
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1228	0.1226	0.001973
0.2487	0.2481	0.002319
0.4603	0.4590	0.002760
0.5592	0.5576	0.002924
0.6717	0.6696	0.003058
0.8367	0.8341	0.003120
0.9228	0.9199	0.003106
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1600	0.1596	0.002351
0.2834	0.2827	0.002616
0.4881	0.4866	0.002972
0.5878	0.5860	0.003103
0.7075	0.7052	0.003186
0.8531	0.8504	0.003155
0.9277	0.9248	0.003125
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1006	0.1004	0.002009
0.1992	0.1987	0.002367
0.3871	0.3860	0.002854
0.4818	0.4803	0.003032
0.5895	0.5877	0.003121
0.7854	0.7829	0.003120
0.8929	0.8901	0.003110
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1065	0.1063	0.002147
0.2203	0.2198	0.002484
0.4270	0.4258	0.002919
0.5244	0.5228	0.003084
0.6247	0.6228	0.003168
0.8137	0.8111	0.003209
0.9021	0.8993	0.003147
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1399	0.1397	0.001447
0.2729	0.2724	0.001776
0.4915	0.4904	0.002272
0.5779	0.5765	0.002436
0.6710	0.6692	0.002613
0.8537	0.8512	0.002906
0.9285	0.9257	0.002996
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[46]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1477	0.1473	0.002502
0.2738	0.2730	0.002803
0.5032	0.5016	0.003184
0.6050	0.6030	0.003240
0.6959	0.6936	0.003307
0.8604	0.8576	0.003233
0.9305	0.9277	0.003152
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

5.5. Anthracene solubility data in binary alkane + 2-butoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1152	0.1150	0.001748
0.2026	0.2022	0.002092
0.3970	0.3959	0.002726
0.4984	0.4969	0.002952
0.6013	0.5994	0.003188
0.7970	0.7942	0.003526
0.8974	0.8941	0.003642
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1162	0.1160	0.002013
0.2221	0.2216	0.002340
0.4265	0.4253	0.002916
0.5177	0.5161	0.003127
0.6334	0.6313	0.003302
0.8369	0.8339	0.003608
0.9286	0.9252	0.003690
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1061	0.1059	0.002225
0.2312	0.2306	0.002604
0.4565	0.4550	0.003187
0.5513	0.5495	0.003333
0.6293	0.6271	0.003435
0.8453	0.8422	0.003683
0.9243	0.9208	0.003733
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.0917	0.0915	0.002026
0.1736	0.1732	0.002356
0.3516	0.3506	0.002897
0.4437	0.4423	0.003092
0.5532	0.5514	0.003282
0.7600	0.7573	0.003532
0.8636	0.8605	0.003655
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1210	0.1207	0.002254
0.2126	0.2120	0.002560
0.4039	0.4027	0.003035
0.5074	0.5058	0.003248
0.6058	0.6038	0.003342
0.8149	0.8120	0.003576
0.9037	0.9004	0.003679
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]

Original Measurements:

[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.0977	0.0976	0.001389
0.2275	0.2271	0.001747
0.4395	0.4385	0.002348
0.5470	0.4555	0.002659
0.6370	0.6352	0.002864
0.8417	0.8389	0.003376
0.9188	0.9155	0.003551
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) *tert*-butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]
(3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]

Original Measurements:

[47]C. E. Hernández, L. E. Roy, G. D. Reddy, G. L. Martinez, A. Parker, A. Jackson, G. Brown, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 1249 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1313	0.1310	0.002522
0.2591	0.2583	0.002896
0.4588	0.4573	0.003317
0.5696	0.5676	0.003512
0.6725	0.6700	0.003662
0.8348	0.8317	0.003770
0.9273	0.9238	0.003780
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

5.6. Anthracene solubility data in binary alkane + 3-methoxy-1-butanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Hexane; C_6H_{14}; [110-54-3] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in hexane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1175	0.1173	0.001696
0.2440	0.2435	0.002079
0.4481	0.4469	0.002576
0.5596	0.5580	0.002785
0.6554	0.6535	0.002893
0.8271	0.8247	0.002889
0.9141	0.9115	0.002803
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in heptane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1216	0.1214	0.002009
0.2596	0.2590	0.002337
0.4640	0.4627	0.002705
0.5653	0.5637	0.002878
0.6659	0.6639	0.002964
0.8421	0.8396	0.002933
0.9125	0.9099	0.002863
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Octane; C_8H_{18}; [111-65-9] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in octane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1406	0.1403	0.002288
0.2681	0.2674	0.002542
0.4926	0.4912	0.002921
0.5954	0.5936	0.003045
0.6860	0.6839	0.003079
0.8435	0.8409	0.003040
0.9102	0.9075	0.002936
0.9287	0.9260	0.002905
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001533
0.0919	0.0917	0.001991
0.2033	0.2028	0.002407
0.3865	0.3854	0.002817
0.4914	0.4899	0.002978
0.5915	0.5897	0.003021
0.7926	0.7902	0.002969
0.8827	0.8802	0.002870
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methylcyclohexane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1251	0.1248	0.002234
0.2244	0.2238	0.002522
0.4239	0.4227	0.002911
0.5353	0.5336	0.003104
0.6258	0.6238	0.003156
0.8104	0.8079	0.003112
0.9039	0.9012	0.002950
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2,2,4-trimethylpentane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1346	0.1344	0.001465
0.2734	0.2729	0.001780
0.4997	0.4986	0.002238
0.5963	0.5949	0.002414
0.6901	0.6883	0.002578
0.8541	0.8518	0.002741
0.9268	0.9243	0.002739
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[48]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:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in *tert*-butylcyclohexane + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1745	0.1741	0.002564
0.2876	0.2868	0.002808
0.5072	0.5056	0.003116
0.6071	0.6052	0.003179
0.7027	0.7005	0.003200
0.8581	0.8555	0.003039
0.9262	0.9235	0.002899
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

6. Solubility of Anthracene in Binary Alcohol + Chloroalkane Solvent Mixtures

6.1. Critical evaluation of experimental solubility data

Acree and co-workers[49,50] determined the solubility of anthracene in several binary solvent mixtures containing tetrachloromethane and 1-chlorobutane with 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, and 3-methyl-1-butanol at 298.15 K. There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 12 binary alcohol + chloroalkane solvent systems studied are summarized in Table 5, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 5 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.1% to 0.7%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental anthracene solubility data for binary alcohol + 1-chlorobutane and alcohol + tetrachloromethane solvent mixtures are given in Secs. 6.2 and 6.3.

TABLE 5. Mathematical representation of anthracene solubilities in binary alcohol (2) + chloroalkane (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
1-Propanol (2) + 1-chlorobutane (3)	1.915	0.7
	0.055	
	0.438	
2-Propanol (2) + 1-chlorobutane (3)	2.244	0.3
	0.698	
	0.189	
1-Butanol (2) + 1-chlorobutane (3)	1.354	0.2
	−0.186	
	0.210	
2-Butanol (2) + 1-chlorobutane (3)	1.819	0.4
	0.570	
2-Methyl-1-propanol (2) + 1-chlorobutane (3)	1.881	0.4
	0.218	
	0.281	
3-Methyl-1-butanol (2) + 1-chlorobutane (3)	1.229	0.4
	−0.228	
	0.199	
1-Propanol (2) + tetrachloromethane (3)	1.322	0.5
	−0.551	
	−0.202	
2-Propanol (2) + tetrachloromethane (3)	1.909	0.5
	−0.413	
	−0.285	
1-Butanol (2) + tetrachloromethane (3)	0.724	0.5
	−0.780	
	−0.064	
2-Butanol (2) + tetrachloromethane (3)	1.372	0.1
	−0.251	
	0.136	
2-Methyl-1-propanol (2) + tetrachloromethane (3)	1.329	0.5
	−0.539	
	−0.037	
3-Methyl-1-butanol (2) + tetrachloromethane (3)	0.773	0.4
	−0.636	
	−0.082	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only two coefficients are listed, then $S_{23,2}$ is zero.
[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

6.2. Anthracene solubility data in binary alcohol + 1-chlorobutane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[49] K. M. De Fina, T. Chee, A. Delacruz, A. Frizzelle, K. Theeuwes, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 499 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 1-chlorobutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0731	0.0730	0.000813
0.1555	0.1553	0.001126
0.3173	0.3167	0.001902
0.4139	0.4129	0.002451
0.5158	0.5142	0.003093
0.7338	0.7304	0.004631
0.8610	0.8563	0.005514
1.0000	0.9941	0.005863

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

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

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99.5+%, HPLC grade, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [57-63-0] (3) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[49]K. M. De Fina, T. Chee, A. Delacruz, A. Frizzelle, K. Theeuwes, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 499 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 1-chlorobutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0805	0.0805	0.000635
0.1549	0.1548	0.000890
0.3197	0.3192	0.001667
0.4269	0.4259	0.002262
0.5299	0.5284	0.002909
0.7374	0.7342	0.004291
0.8571	0.8528	0.005011
1.0000	0.9941	0.005863

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

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

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99.5+%, HPLC grade, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[49]K. M. De Fina, T. Chee, A. Delacruz, A. Frizzelle, K. Theeuwes, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 499 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 1-chlorobutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0942	0.0941	0.001085
0.1903	0.1900	0.001429
0.3633	0.3625	0.002234
0.4660	0.4647	0.002830
0.5578	0.5559	0.003428
0.7581	0.7545	0.004781
0.8696	0.8649	0.005421
1.0000	0.9941	0.005863

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99.5+%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[49]K. M. De Fina, T. Chee, A. Delacruz, A. Frizzelle, K. Theeuwes, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 499 (2001).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 1-chlorobutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1013	0.1012	0.000908
0.1830	0.1828	0.001243
0.3546	0.3539	0.002090
0.4685	0.4672	0.002709
0.5766	0.5747	0.003347
0.7704	0.7669	0.004525
0.8708	0.8664	0.005103
1.0000	0.9941	0.005863

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[49]K. M. De Fina, T. Chee, A. Delacruz, A. Frizzelle, K. Theeuwes, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 499 (2001).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 1-chlorobutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0938	0.0937	0.000720
0.1779	0.1777	0.001008
0.3648	0.3641	0.001855
0.4822	0.4810	0.002570
0.5632	0.5615	0.003066
0.7648	0.7614	0.004474
0.8815	0.8768	0.005308
1.0000	0.9941	0.005863

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	[49]K. M. De Fina, T. Chee, A. Delacruz, A. Frizzelle, K. Theeuwes, and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 499 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 1-chlorobutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1061	0.1060	0.001013
0.2037	0.2034	0.001345
0.4165	0.4155	0.002317
0.5132	0.5117	0.002901
0.6148	0.6126	0.003583
0.8018	0.7979	0.004847
0.8844	0.8796	0.005417
1.0000	0.9941	0.005863

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

6.3. Anthracene solubility data in binary alcohol + tetrachloromethane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Tetrachloromethane; CCl_4; [75-05-8]	[50]P. G. Taylor, A. M. Tran, A. K. Charlton, D. R. Daniels, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1603 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + tetrachloromethane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0962	0.0961	0.000770
0.1768	0.1766	0.000965
0.3363	0.3358	0.001499
0.4363	0.4354	0.001975
0.5579	0.5564	0.002651
0.7650	0.7621	0.003756
0.8485	0.8450	0.004163
1.0000	0.9954	0.004622

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Propanol; C_3H_8O; [57-63-0]
(3) Tetrachloromethane; CCl_4; [75-05-8]

Original Measurements:
[50]P. G. Taylor, A. M. Tran, A. K. Charlton, D. R. Daniels, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1603 (2003).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + tetrachloromethane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0947	0.0946	0.000581
0.1836	0.1835	0.000809
0.3447	0.3442	0.001406
0.4340	0.4332	0.001871
0.5843	0.5827	0.002703
0.7524	0.7496	0.003696
0.8736	0.8699	0.004284
1.0000	0.9954	0.004622

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]
(3) Tetrachloromethane; CCl_4; [75-05-8]

Original Measurements:
[50]P. G. Taylor, A. M. Tran, A. K. Charlton, D. R. Daniels, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1603 (2003).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + tetrachloromethane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0983	0.0982	0.000953
0.1950	0.1948	0.001178
0.3955	0.3948	0.001833
0.4886	0.4875	0.002236
0.5864	0.5848	0.002768
0.7894	0.7864	0.003844
0.8969	0.8930	0.004364
1.0000	0.9954	0.004622

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]
(3) Tetrachloromethane; CCl_4; [75-05-8]

Original Measurements:
[50]P. G. Taylor, A. M. Tran, A. K. Charlton, D. R. Daniels, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1603 (2003).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + tetrachloromethane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1231	0.1230	0.000863
0.2070	0.2068	0.001109
0.3943	0.3936	0.001815
0.4872	0.4861	0.002252
0.5925	0.5908	0.002802
0.7912	0.7881	0.003882
0.8834	0.8796	0.004306
1.0000	0.9954	0.004622

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Tetrachloromethane; CCl_4; [75-05-8]	[50]P. G. Taylor, A. M. Tran, A. K. Charlton, D. R. Daniels, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1603 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + tetrachloromethane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1281	0.1280	0.000696
0.2088	0.2086	0.000897
0.3831	0.3825	0.001489
0.4950	0.4940	0.002049
0.6027	0.6011	0.002627
0.7893	0.7864	0.003718
0.8936	0.8898	0.004283
1.0000	0.9954	0.004622

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99.5%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Tetrachloromethane; CCl_4; [75-05-8]	[50]P. G. Taylor, A. M. Tran, A. K. Charlton, D. R. Daniels, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1603 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + tetrachloromethane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1181	0.1180	0.000926
0.2261	0.2258	0.001187
0.4333	0.4325	0.001927
0.5339	0.5326	0.002390
0.6336	0.6317	0.002922
0.8162	0.8130	0.003864
0.9003	0.8964	0.004312
1.0000	0.9954	0.004622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99.5%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K

$x_3^{(s)}$: ±0.0001

x_1: ±1.0% (relative error).

7. Solubility of Anthracene in Binary Alcohol + Ether Solvent Mixtures

7.1. Critical evaluation of experimental solubility data

Acree and co-workers[51–55] have measured the solubility of anthracene in binary alcohol + 1,4-dioxane, alcohol + 1,1′-oxybisbutane, alcohol + 2-methoxy-2-methylpropane (also called methyl *tert*-butyl ether), and 1,1′-oxybis[2-methoxyethane] solvent mixtures at 298.2 K. The alcohol solvents included 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 3-methyl-1-butanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, and 1-octanol. There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 35 binary alcohol + ether solvent systems studied are summarized in Table 6, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 6 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 2.3%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental anthracene solubility data for binary alcohol + 1,4-dioxane, alcohol + 1,1′-oxybisbutane, alcohol + 2,2′-oxybispropane, alcohol + 2-methoxy-2-methylpropane, and alcohol + 1,1′-oxybis[2-methoxyethane] solvent mixtures are given in Secs. 7.2–7.6.

TABLE 6. Mathematical representation of anthracene solubilities in binary alcohol (2) + ether (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
1-Propanol (2) + 1,4-dioxane (3)	2.308	0.8
	1.305	
	0.112	
2-Propanol (2) + 1,4-dioxane (3)	2.559	0.8
	1.745	
	0.748	
1-Butanol (2) + 1,4-dioxane (3)	1.792	0.7
	1.140	
	−0.330	
2-Butanol (2) + 1,4-dioxane (3)	2.178	0.9
	1.504	
	0.709	
2-Methyl-1-propanol (2) + 1,4-dioxane (3)	2.326	0.5
	1.232	
	0.210	
3-Methyl-1-butanol (2) + 1,4-dioxane (3)	1.773	0.3
	0.627	
	0.366	
1-Octanol (2) + 1,4-dioxane (3)	0.968	0.5
	0.034	
	0.174	
1-Propanol (2) + 1,1′-oxybisbutane (3)	2.167	1.1
	0.931	
	0.891	
2-Propanol (2) + 1,1′-oxybisbutane (3)	2.588	0.8
	1.235	
	0.866	
1-Butanol (2) + 1,1′-oxybisbutane (3)	1.736	0.9
	0.488	
	0.574	
2-Butanol (2) + 1,1′-oxybisbutane (3)	2.109	0.3
	0.849	
	0.726	
2-Methyl-1-propanol (2) + 1,1′-oxybisbutane (3)	2.231	0.6
	0.932	
	0.929	
3-Methyl-1-butanol (2) + 1,1′-oxybisbutane (3)	1.694	0.3
	0.464	
	0.338	
1-Octanol (2) + 1,1′-oxybisbutane (3)	0.712	0.6
	−0.143	
	0.169	
1-Propanol (2) + 2,2′-oxybispropane (3)	1.950	0.6
	0.665	
	0.907	
2-Propanol (2) + 2,2′-oxybispropane (3)	2.200	1.1
	0.853	
	1.097	
1-Butanol (2) + 2,2′-oxybispropane (3)	1.624	0.8
	0.484	
	0.829	
2-Butanol (2) + 2,2′-oxybispropane (3)	1.855	0.5
	0.501	
	0.689	
2-Methyl-1-propanol (2) + 2,2′-oxybispropane (3)	2.034	0.4
	−0.592	
	0.636	
3-Methyl-1-butanol (2) + 2,2′-oxybispropane (3)	1.565	0.4
	0.377	
	0.640	
1-Propanol (2) + 2-methoxy-2-methylpropane (3)	1.688	0.2
	0.283	
	0.272	

TABLE 6. Mathematical representation of anthracene solubilities in binary alcohol (2) + ether (3) solvent mixtures—Continued

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
2-Propanol (2) + 2-methoxy-2-methylpropane (3)	1.976	0.5
	0.514	
	0.651	
1-Butanol (2) + 2-methoxy-2-methylpropane (3)	1.305	0.2
	0.190	
	0.282	
2-Butanol (2) + 2-methoxy-2-methylpropane (3)	1.580	0.3
	0.272	
	0.294	
2-Methyl-1-propanol (2) + 2-methoxy-2-methylpropane (3)	1.652	0.4
	0.428	
	0.353	
1-Pentanol (2) + 2-methoxy-2-methylpropane (3)	1.003	0.2
	−0.033	
	0.244	
3-Methyl-1-butanol (2) + 2-methoxy-2-methylpropane (3)	1.196	0.3
	0.204	
	0.256	
1-Octanol (2) + 2-methoxy-2-methylpropane (3)	0.841	0.4
	0.092	
	0.449	
1-Propanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.704	1.1
	1.905	
	1.609	
2-Propanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	3.099	2.3
	2.363	
	2.555	
1-Butanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.182	1.4
	1.531	
	1.185	
2-Butanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.740	1.1
	1.826	
	1.221	
2-Methyl-1-pentanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	1.958	0.5
	1.012	
	0.504	
4-Methyl-2-pentanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	2.125	0.5
	1.182	
	0.556	
1-Octanol (2) + 1,1′-oxybis[2-methoxyethane] (3)	1.232	0.8
	0.466	
	0.407	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\text{exp}} - x_1^{\text{cal}}]/x_1^{\text{exp}}\ |$.

7.2. Anthracene solubility data in binary alcohol + 1,4-dioxane solvent mixtures

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]	[51] J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0939	0.0938	0.001016
0.1829	0.1826	0.001525
0.3631	0.3621	0.002778
0.3717	0.3703	0.003687
0.5753	0.5727	0.004482
0.7832	0.7783	0.006214
0.8978	0.8914	0.007182
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

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

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99.8%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.8% (relative error).

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]	[51] J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.1009	0.1008	0.000836
0.1879	0.1877	0.001308
0.3756	0.3746	0.002559
0.4768	0.4752	0.003349
0.5313	0.5293	0.003811
0.7806	0.7760	0.005852
0.8863	0.8801	0.006990
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]	[51] J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1160	0.1158	0.001358
0.2039	0.2035	0.001888
0.4189	0.4175	0.003408
0.5175	0.5154	0.004154
0.6260	0.6229	0.004947
0.8022	0.7972	0.006205
0.9022	0.8959	0.006983
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]	[51] J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1116	0.1115	0.001153
0.2209	0.2205	0.001815
0.4277	0.4263	0.003287
0.5135	0.5115	0.003948
0.6189	0.6160	0.004764
0.8101	0.8050	0.006284
0.9012	0.8946	0.007304
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]	[51]J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1125	0.1124	0.000915
0.2170	0.2167	0.001478
0.4216	0.4204	0.002896
0.5209	0.5190	0.003704
0.6243	0.6214	0.004583
0.8166	0.8114	0.006328
0.9250	0.9182	0.007392
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]	[51]J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1272	0.1270	0.001300
0.2448	0.2443	0.001977
0.4633	0.4616	0.003574
0.5625	0.5601	0.004350
0.6549	0.6515	0.005131
0.8172	0.8117	0.006694
0.9072	0.9004	0.007547
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]
(3) 1,4-Dioxane; $C_4H_4O_2$; [123-91-1]

Original Measurements:
[51]J. R. Powell, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1124 (1995).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 1,4-dioxane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1825	0.1819	0.003215
0.3107	0.3094	0.004060
0.5599	0.5566	0.005816
0.6485	0.6443	0.006519
0.7328	0.7276	0.007063
0.8775	0.8705	0.007998
0.9429	0.9352	0.008177
1.0000	0.9917	0.008329

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

7.3. Anthracene solubility data in binary alcohol + 1,1′-oxybisbutane solvent mixtures

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Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Propanol; C_3H_8O; [71-23-8]
(3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

Original Measurements:
[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0532	0.0532	0.000787
0.0984	0.0983	0.000961
0.2230	0.2227	0.001463
0.3074	0.3069	0.001784
0.3948	0.3939	0.002175
0.6368	0.6349	0.003018
0.8042	0.8015	0.003409
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Propanol; C_3H_8O; [67-63-0]
(3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

Original Measurements:
[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0517	0.0517	0.000570
0.1101	0.1100	0.000750
0.2268	0.2265	0.001226
0.3126	0.3121	0.001609
0.4412	0.4403	0.001989
0.6286	0.6268	0.002827
0.7938	0.7912	0.003267
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]
(3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

Original Measurements:

[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0564	0.0563	0.001004
0.1215	0.1213	0.001246
0.2719	0.3714	0.001822
0.3541	0.3534	0.002085
0.4627	0.4615	0.002513
0.6851	0.6829	0.003259
0.8369	0.8339	0.003526
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]
(3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

Original Measurements:

[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0642	0.0641	0.000807
0.1203	0.1202	0.001019
0.2536	0.2532	0.001544
0.3457	0.3450	0.001901
0.3916	0.3908	0.002085
0.6777	0.6756	0.003067
0.7413	0.7389	0.003211
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0627	0.0627	0.000668
0.1127	0.1126	0.000837
0.2427	0.2424	0.001323
0.3429	0.3423	0.001693
0.4450	0.4441	0.002093
0.6767	0.6747	0.002936
0.8164	0.8137	0.003345
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [71-23-8] (3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0753	0.0752	0.000964
0.1270	0.1269	0.001142
0.2884	0.2879	0.001737
0.3892	0.3884	0.002076
0.4656	0.4645	0.002350
0.6713	0.6693	0.003026
0.7950	0.7923	0.003343
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[52]J. R. Powell and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 914 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 1,1′-oxybisbutane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.0964	0.0962	0.002415
0.1982	0.1977	0.002665
0.3832	0.3820	0.003114
0.4861	0.4845	0.003299
0.5892	0.5872	0.003459
0.7847	0.7817	0.003792
0.8897	0.8864	0.003722
1.0000	0.9964	0.003615

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

7.4. Anthracene solubility data in binary alcohol + 2,2′-oxybispropane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[53]M. Corrella, K. Wolcott, M. Carrillo, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 929 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0649	0.0648	0.000793
0.1171	0.1170	0.000949
0.2663	0.2659	0.001388
0.3333	0.3328	0.001638
0.4519	0.4501	0.001900
0.6433	0.6418	0.002302
0.8166	0.8146	0.002549
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[53]M. Corrella, K. Wolcott, M. Carrillo, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 929 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0551	0.0551	0.000559
0.1147	0.1146	0.000713
0.2631	0.2628	0.001139
0.3560	0.3555	0.001387
0.4948	0.4939	0.001777
0.6336	0.6323	0.002115
0.8201	0.8181	0.002454
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[53]M. Corrella, K. Wolcott, M. Carrillo, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 929 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0797	0.0796	0.001068
0.1443	0.1441	0.001261
0.2974	0.2969	0.001677
0.3966	0.2958	0.001914
0.4952	0.4941	0.002143
0.7263	0.7245	0.002544
0.8363	0.8342	0.002605
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[53]M. Corrella, K. Wolcott, M. Carrillo, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 929 (2007).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0812	0.0811	0.000811
0.1584	0.1582	0.001027
0.3032	0.3027	0.001535
0.3953	0.3946	0.001661
0.5090	0.5080	0.001963
0.7448	0.7430	0.002449
0.8438	0.8417	0.002539
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[53]M. Corrella, K. Wolcott, M. Carrillo, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 929 (2007).

Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0696	0.0696	0.000644
0.1434	0.1433	0.000836
0.3193	0.3189	0.001323
0.3941	0.3935	0.001538
0.5031	0.5021	0.001834
0.7176	0.7160	0.002299
0.8561	0.8540	0.002505
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[53]M. Corrella, K. Wolcott, M. Carrillo, and W. E. Acree, Jr., J. Chem. Eng. Data **52**, 929 (2007).

Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2,2′-oxybispropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0955	0.0954	0.001001
0.1765	0.1763	0.001251
0.3343	0.3338	0.001629
0.4307	0.4299	0.001842
0.5258	0.5247	0.002066
0.7552	0.7533	0.002478
0.8738	0.8716	0.002571
1.0000	0.9975	0.002515

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from acetone.
(2) 99%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

7.5. Anthracene solubility data in binary alcohol + 2-methoxy-2-methylpropane solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0653	0.0653	0.000750
0.1335	0.1334	0.000931
0.2757	0.2753	0.001348
0.3818	0.3812	0.001684
0.4847	0.4837	0.001992
0.7110	0.7091	0.002659
0.8378	0.8354	0.002908
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0714	0.0714	0.000574
0.1398	0.1397	0.000755
0.2795	0.2792	0.001156
0.3931	0.3925	0.001487
0.4865	0.4856	0.001777
0.7224	0.7205	0.002571
0.8513	0.8488	0.002885
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0817	0.0816	0.001013
0.1574	0.1572	0.001216
0.3364	0.3358	0.001710
0.4375	0.4366	0.001992
0.5403	0.5391	0.002282
0.7522	0.7501	0.002790
0.8598	0.8573	0.002957
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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) HPLC grade, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0838	0.0837	0.000783
0.1593	0.1591	0.000985
0.3367	0.3362	0.001490
0.4388	0.4380	0.001793
0.5316	0.5305	0.002068
0.7485	0.7465	0.002695
0.8667	0.8642	0.002918
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0757	0.0757	0.000636
0.1665	0.1664	0.000854
0.3386	0.3382	0.001324
0.4145	0.4139	0.001562
0.5376	0.5366	0.001928
0.7484	0.7465	0.002549
0.8554	0.8530	0.002804
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

(3) 99.9+%, Arco Chemical Company, USA.

Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.0724	0.0723	0.001326
0.1686	0.1683	0.001518
0.3791	0.3783	0.002061
0.4028	0.4019	0.002248
0.5784	0.5770	0.002542
0.7225	0.7204	0.002921
0.8892	0.8865	0.003061
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

(3) 99.9+%, Arco Chemical Company, USA.

Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0914	0.0913	0.000942
0.1886	0.1884	0.001185
0.3569	0.3563	0.001613
0.4803	0.4794	0.001954
0.5377	0.5365	0.002219
0.7795	0.7774	0.002725
0.8882	0.8856	0.002919
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[54]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 1215 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-methoxy-2-methylpropane mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1364	0.1360	0.002586
0.2405	0.2398	0.002840
0.4577	0.4563	0.003107
0.5516	0.5498	0.003193
0.6647	0.6625	0.003310
0.8384	0.8356	0.003305
0.9187	0.9158	0.003210
1.0000	0.9969	0.003050

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined 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%, anhydrous, Aldrich Chemical Company.
(3) 99.9+%, Arco Chemical Company, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

7.6. Anthracene solubility data in binary alcohol + 1,1′-oxybis[2-methoxyethane] solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0557	0.0556	0.000944
0.1183	0.1181	0.001417
0.2497	0.2401	0.002575
0.3374	0.3362	0.003505
0.4300	0.4281	0.004439
0.6676	0.6628	0.00718
0.8129	0.9910	0.00897
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0603	0.0603	0.000764
0.1186	0.1185	0.001158
0.2606	0.2600	0.002423
0.3508	0.3497	0.003253
0.4473	0.4454	0.004323
0.6810	0.6762	0.00712
0.8122	0.8049	0.00895
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0722	0.0721	0.001302
0.1402	0.1399	0.001848
0.2984	0.2974	0.003304
0.3937	0.3920	0.004301
0.5218	0.5191	0.00524
0.7254	0.7196	0.00794
0.8440	0.8361	0.00934
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0659	0.0658	0.000983
0.1294	0.1292	0.001478
0.2930	0.2021	0.002940
0.3785	0.3770	0.003843
0.4973	0.4947	0.00518
0.7261	0.7204	0.00788
0.8480	0.8400	0.00939
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-pentanol; C_6H_{14}; [105-30-6] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-pentanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000966
0.0944	0.0942	0.001592
0.1793	0.1789	0.002278
0.3576	0.3562	0.003925
0.4536	0.4514	0.004901
0.5709	0.5674	0.00617
0.7659	0.7593	0.00859
0.8783	0.8697	0.00983
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (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] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 4-methyl-2-pentanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000779
0.0960	0.0959	0.001363
0.1758	0.1755	0.001954
0.3693	0.3679	0.003697
0.4736	0.4713	0.004801
0.5747	0.5713	0.00590
0.7690	0.7626	0.00828
0.8825	0.8739	0.00972
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, Acros Organics.
(3) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 1,1′-Oxybis[2-methoxyethane]; $C_6H_{14}O_3$; [111-96-6]	[55]J. R. Powell, K. S. Coym, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 395 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 1,1′-oxybis[2-methoxyethane] mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1198	0.1194	0.003209
0.2208	0.2207	0.004063
0.4248	0.4222	0.00606
0.5226	0.5189	0.00703
0.6205	0.6155	0.00798
0.8001	0.7924	0.00959
0.8967	0.8871	0.01069
1.0000	0.9886	0.01139

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.8% (relative error).

8. Solubility of Anthracene in Binary Alcohol + Alcohol Solvent Mixtures

8.1. Critical evaluation of experimental solubility data

Volume 58 in the IUPAC Solubility Data Series[2] contained solubility data for anthracene in binary 1-butanol + 1-propanol, 2-butanol + 1-propanol, 2-propanol + 1-propanol, 1-octanol + 1-propanol, 1-butanol + 2-propanol, 2-butanol + 2-propanol, and 1-octanol + 2-butanol solvent mixtures at 298.15 K. To conserve space, data from the earlier volume will not be repeated in this volume. Attention will be focused on compiling experimental values determined after Vol. 58 was published.

Acree and co-workers[56–60] reported the solubility of anthracene in several binary alcohol + alcohol solvent systems at 298.15 K. The solvents included nine primary alcohols (1-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 2-methyl-1-pentanol, 1-octanol, and 2-ethyl-1-hexanol) and four secondary alcohols (2-propanol, 2-butanol, 2-pentanol, 4-methyl-2-pentanol). There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 37 binary alcohol + alcohol solvent systems studied are summarized in Table 7, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 7 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 0.7%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

Solubility data are arranged according to alcohol type. The experimental anthracene solubility data for binary primary alcohol + primary alcohol, primary alcohol + secondary alcohol solvent mixtures, and secondary alcohol + secondary alcohol solvent mixtures are given in Secs. 8.2–8.4.

TABLE 7. Mathematical representation of anthracene solubilities in binary alcohol (2) + alcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
1-Propanol (2) + 2-methyl-1-butanol (3)	0.031	0.3
	0.267	
	0.174	
2-Propanol (2) + 2-methyl-1-butanol (3)	0.154	0.7
	0.509	
	0.162	
1-Butanol (2) + 2-methyl-1-butanol (3)	0.000	0.2
2-Butanol (2) + 2-methyl-1-butanol (3)	−0.040	0.7
	0.433	
	0.021	
2-Methyl-1-propanol (2) + 2-methyl-1-butanol (3)	−0.024	0.4
	0.123	
3-Methyl-1-butanol (2) + 2-methyl-1-butanol (3)	−0.034	0.2
	0.035	
2-Pentanol (2) + 2-methyl-1-butanol (3)	0.000	0.4
3-Methyl-1-butanol (2) + 2-butanol (3)	0.093	0.8
	0.087	
2-Butanol (2) + 2-methyl-1-propanol (3)	0.000	0.3
1-Octanol (2) + 2-methyl-1-propanol (3)	0.940	0.5
	−0.340	
	0.341	
3-Methyl-1-butanol (2) + 1-butanol (3)	0.065	0.4
3-Methyl-1-butanol (2) + 2-methyl-1-propanol (3)	0.124	0.2
	−0.041	
3-Methyl-1-butanol (2) + 1-octanol (3)	0.467	0.3
	0.166	
1-Propanol (2) + 2-methyl-1-propanol (3)	0.078	0.4
	−0.019	
2-Methyl-1-proapnol (2) + 2-propanol (3)	0.098	0.2
	0.014	
3-Methyl-1-butanol (2) + 2-propanol (3)	0.236	0.2
	0.036	
1-Propanol (2) + 2-pentanol (3)	0.000	0.3
2-Propanol (2) + 2-pentanol (3)	0.216	0.4
	0.134	
1-Butanol (2) + 2-pentanol (3)	0.000	0.3
2-Butanol (2) + 2-pentanol (3)	0.000	0.3
2-Methyl-1-propanol (2) + 2-pentanol (3)	0.059	0.4
1-Pentanol (2) + 2-pentanol (3)	0.000	0.5
3-Methyl-1-butanol (2) + 2-pentanol (3)	0.034	0.3
1-Octanol (1) + 2-pentanol (3)	0.497	0.3
	−0.089	
	0.179	
1-Propanol (2) + 4-methyl-2-pentanol (3)	−0.045	0.7
	0.119	
2-Propanol (2) + 4-methyl-2-pentanol (3)	0.106	0.4
	0.123	
	0.095	
1-Butanol (2) + 4-methyl-2-pentanol (3)	−0.097	0.2
	−0.077	
2-Butanol (2) + 4-methyl-2-pentanol (3)	0.060	0.2
2-Methyl-1-propanol (2) + 4-methyl-2-pentanol (3)	0.064	0.2
1-Pentanol (2) + 4-methyl-2-pentanol (3)	−0.103	0.4
	0.056	
	0.141	
3-Methyl-1-butanol (2) + 4-methyl-2-pentanol (3)	0.042	0.3
1-Octanol (1) + 4-methyl-2-pentanol (3)	0.379	0.3
	0.028	
	0.566	
1-Propanol (2) + 1-pentanol (3)	0.216	0.2
	0.089	
	−0.104	
2-Propanol (2) + 1-pentanol (3)	0.445	0.3
	0.111	
	0.033	
1-Butanol (2) + 1-pentanol (3)	0.055	0.2
	0.033	
	−0.016	
2-Butanol (2) + 1-pentanol (3)	0.106	0.3
	−0.054	
	−0.035	
2-Methyl-1-propanol (2) + 1-pentanol (3)	0.267	0.3
	0.044	
	0.078	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only a single coefficient is listed, then $S_{23,1}$ and $S_{23,2}$ are zero. Similarly, if two coefficients are listed, then $S_{23,2}$ is zero.

[b] Dev (%) = $(100/N)\,\Sigma\,|\,[x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\,|$.

8.2. Anthracene solubility data in binary primary alcohol + primary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[56] A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0933	0.0932	0.000584
0.1757	0.1756	0.000572
0.3481	0.3479	0.000552
0.4479	0.4477	0.000540
0.5554	0.5551	0.000529
0.7554	0.7550	0.000504
0.8733	0.8729	0.000491
1.0000	0.9995	0.000470

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[57]C. I. Monárrez, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1341 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0901	0.0900	0.000623
0.1537	0.1536	0.000646
0.3090	0.3088	0.000666
0.4030	0.4027	0.000669
0.5214	0.5210	0.000689
0.7294	0.7289	0.000715
0.8209	0.8203	0.000742
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[57]C. I. Monárrez, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1341 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0885	0.0884	0.000801
0.1869	0.1867	0.000803
0.3816	0.3813	0.000795
0.4621	0.4621	0.000795
0.5861	0.5856	0.000793
0.7789	0.7782	0.000791
0.8742	0.8735	0.000789
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[57]C. I. Monárrez, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1341 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1074	0.1073	0.000512
0.1916	0.1915	0.000541
0.3689	0.3687	0.000574
0.4513	0.4510	0.000593
0.5616	0.5613	0.000617
0.7692	0.7687	0.000673
0.8860	0.8854	0.000714
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99.5%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0752	0.0752	0.000627
0.1490	0.1489	0.000668
0.3170	0.3168	0.000756
0.4120	0.4117	0.000806
0.5165	0.5161	0.000859
0.7217	0.7210	0.000950
0.8590	0.8581	0.001020
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0944	0.0943	0.000833
0.1791	0.1789	0.000854
0.3634	0.3631	0.000914
0.4608	0.4604	0.000932
0.5455	0.5450	0.000969
0.7716	0.7709	0.001027
0.8926	0.8917	0.001061
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	**Original Measurements:** [58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0929	0.0929	0.000525
0.1818	0.1817	0.000576
0.3594	0.3592	0.000678
0.4476	0.4473	0.000735
0.5685	0.5680	0.000814
0.7699	0.7692	0.000946
0.8800	0.8791	0.001019
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	**Original Measurements:** [58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1127	0.1126	0.000775
0.1969	0.1967	0.000799
0.3941	0.3938	0.000863
0.4977	0.4973	0.000894
0.7067	0.7060	0.000969
0.7944	0.7936	0.001020
0.8938	0.8929	0.001054
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]
(3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:

[58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1466	0.1463	0.002026
0.2735	0.2730	0.001893
0.4864	0.4856	0.001648
0.5878	0.5869	0.001550
0.6852	0.6842	0.001440
0.8469	0.8458	0.001257
0.9244	0.9233	0.001179
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]

Original Measurements:

[57]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; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1215	0.1212	0.000733
0.2037	0.2035	0.000739
0.3955	0.3952	0.000743
0.5037	0.5033	0.000748
0.6169	0.6164	0.000756
0.7935	0.7929	0.000766
0.8880	0.8873	0.000775
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1766	0.1763	0.001872
0.3099	0.3094	0.001617
0.5312	0.5306	0.001219
0.6295	0.6288	0.001056
0.7215	0.7204	0.000901
0.8697	0.8691	0.000670
0.9351	0.9346	0.000568
1.0000	0.9995	0.000470

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0810	0.0809	0.000830
0.1578	0.1577	0.000933
0.3162	0.3158	0.001155
0.4024	0.4019	0.001269
0.5109	0.5102	0.001425
0.7229	0.7217	0.001718
0.8415	0.8399	0.001910
1.0000	0.9978	0.002160

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1375	0.1374	0.000692
0.2373	0.2371	0.000668
0.4385	0.4382	0.000618
0.5407	0.5404	0.000592
0.6456	0.6452	0.000567
0.8175	0.8171	0.000523
0.8981	0.8977	0.000497
1.0000	0.9995	0.000470

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1294	0.1293	0.000745
0.2385	0.2383	0.000751
0.4402	0.4399	0.000768
0.5442	0.5438	0.000775
0.6471	0.6466	0.000781
0.8112	0.8106	0.000793
0.9031	0.9024	0.000801
1.0000	0.9992	0.000801

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [67-63-0] (3) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[59]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-methyl-1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0737	0.0737	0.000626
0.1347	0.1346	0.000654
0.2837	0.2835	0.000713
0.3727	0.3724	0.000748
0.4557	0.4553	0.000771
0.7050	0.7044	0.000851
0.8395	0.8387	0.000897
1.0000	0.9990	0.000966

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[59]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables: *T*/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-methyl-1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0865	0.0865	0.000813
0.1692	0.1691	0.000824
0.3256	0.3253	0.000848
0.4476	0.4472	0.000866
0.5278	0.5273	0.000879
0.7486	0.7479	0.000916
0.8606	0.8598	0.000939
1.0000	0.9990	0.000966

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[59]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables: *T*/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-methyl-1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0865	0.0865	0.000516
0.1575	0.1574	0.000549
0.3292	0.3290	0.000631
0.4334	0.4331	0.000678
0.5354	0.5350	0.000724
0.7468	0.7462	0.000827
0.8653	0.8645	0.000893
1.0000	0.9990	0.000966

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[59]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-methyl-1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1359	0.1356	0.001953
0.2390	0.2386	0.001844
0.4525	0.4518	0.001571
0.5583	0.5575	0.001448
0.6387	0.6378	0.001354
0.8279	0.8270	0.001122
0.9165	0.9155	0.001047
1.0000	0.9990	0.000966

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

8.3. Anthracene solubility data in binary primary alcohol + secondary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[57]C. I. Monárrez, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 1341 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0931	0.0931	0.000467
0.1659	0.1658	0.000491
0.3264	0.3262	0.000545
0.4298	0.4296	0.000576
0.5216	0.5213	0.000601
0.7443	0.7438	0.000662
0.8572	0.8566	0.000701
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]
(3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]

Original Measurements:
[57]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0862	0.0861	0.000618
0.1784	0.1783	0.000637
0.3684	0.3682	0.000659
0.4613	0.4610	0.000667
0.5584	0.5580	0.000683
0.7708	0.7703	0.000709
0.8895	0.8889	0.000730
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]
(3) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]

Original Measurements:
[57]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-pentanol + 2-methyl-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000800
0.1032	0.1031	0.000808
0.2144	0.2142	0.000800
0.4011	0.4008	0.000795
0.5105	0.5100	0.000795
0.6114	0.6109	0.000792
0.7899	0.7893	0.000790
0.9010	0.9003	0.000789
1.0000	0.9992	0.000786

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized three times from acetone.
(2) 99+%, Acros Organics, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]
(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

Original Measurements:
[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000800
0.1118	0.1117	0.000573
0.2077	0.2076	0.000558
0.3966	0.3964	0.000534
0.4964	0.4961	0.000524
0.6002	0.5999	0.000513
0.7892	0.7888	0.000494
0.8840	0.8836	0.000484
1.0000	0.9995	0.000470

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Propanol; C_3H_8O; [67-63-0]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1341	0.1340	0.000468
0.2400	0.2399	0.000463
0.4458	0.4456	0.000454
0.5484	0.5482	0.000448
0.6500	0.6497	0.000439
0.8204	0.8201	0.000425
0.8973	0.8969	0.000421
1.0000	0.9996	0.000411

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Propanol; C_3H_8O; [67-63-0]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1561	0.1560	0.000689
0.2741	0.2739	0.000651
0.4809	0.4806	0.000586
0.5887	0.5884	0.000551
0.6833	0.6829	0.000519
0.8398	0.8394	0.000463
0.9209	0.9205	0.000436
1.0000	0.9996	0.000411

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[56]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 917 (1995).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1335	0.1334	0.000725
0.2423	0.2421	0.000703
0.4392	0.4389	0.000672
0.5401	0.5397	0.000655
0.6485	0.6481	0.000635
0.8191	0.8186	0.000620
0.9090	0.9085	0.000597
1.0000	0.9994	0.000585

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[60]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0754	0.0754	0.000605
0.1340	0.1339	0.000617
0.3093	0.3091	0.000650
0.4323	0.4320	0.000679
0.5184	0.5180	0.000693
0.7333	0.7328	0.000737
0.8555	0.8548	0.000763
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]
(3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]

Original Measurements:
[60]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0983	0.0982	0.000797
0.1779	0.1778	0.000803
0.3629	0.3626	0.000804
0.4531	0.4527	0.000800
0.5664	0.5659	0.000798
0.7670	0.7664	0.000802
0.8801	0.8794	0.000796
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]
(3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]

Original Measurements:
[60]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0929	0.0929	0.000497
0.1774	0.1773	0.000525
0.3584	0.3582	0.000575
0.4603	0.4600	0.000607
0.5678	0.5674	0.000645
0.7592	0.7587	0.000706
0.8556	0.8550	0.000745
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]
(3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]

Original Measurements:
[60]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.1438	0.1438	0.001048
0.2514	0.2511	0.001003
0.4638	0.4634	0.000950
0.5418	0.5413	0.000932
0.6137	0.6131	0.000912
0.7819	0.7812	0.000857
0.8761	0.8754	0.000828
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[60] J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1465	0.1464	0.000746
0.2478	0.2476	0.000751
0.4688	0.4684	0.000764
0.5703	0.5699	0.000772
0.6382	0.6377	0.000779
0.7709	0.7703	0.000787
0.9005	0.8998	0.000796
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[60] J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1481	0.1478	0.001989
0.2618	0.2613	0.001841
0.4964	0.4957	0.001485
0.6001	0.5993	0.001348
0.7177	0.7168	0.001191
0.8523	0.8514	0.001007
0.9345	0.9337	0.000891
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[60]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0621	0.0621	0.000606
0.1344	0.1343	0.000617
0.2855	0.2853	0.000635
0.3712	0.3710	0.000645
0.4714	0.4711	0.000660
0.6903	0.6898	0.000699
0.8427	0.8421	0.000740
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[60]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0894	0.0893	0.000787
0.1639	0.1638	0.000781
0.3256	0.3253	0.000777
0.4213	0.4210	0.000775
0.5283	0.5279	0.000771
0.7448	0.7442	0.000773
0.8511	0.8504	0.000778
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]
(3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]

Original Measurements:
[60]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0782	0.0782	0.000492
0.1532	0.1531	0.000513
0.3293	0.3291	0.000563
0.4411	0.4408	0.000596
0.5312	0.5309	0.000624
0.7464	0.7459	0.000694
0.8586	0.8580	0.000728
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]
(3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]

Original Measurements:
[60]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.0988	0.0987	0.001059
0.1781	0.1779	0.001024
0.3605	0.3601	0.000955
0.4934	0.4930	0.000901
0.5579	0.5574	0.000876
0.7586	0.7580	0.000833
0.8682	0.8675	0.000809
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]

Original Measurements:
[60]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0918	0.0917	0.000737
0.1797	0.1796	0.000742
0.3346	0.3343	0.000749
0.5108	0.5104	0.000758
0.6268	0.6263	0.000765
0.7599	0.7593	0.000770
0.8811	0.8804	0.000775
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ± 0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[60]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthraene in 1-octanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1288	0.1285	0.002057
0.2448	0.2443	0.001865
0.4543	0.4536	0.001490
0.5803	0.5795	0.001317
0.6361	0.6353	0.001246
0.8159	0.8151	0.001021
0.9045	0.9037	0.000916
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ± 0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0731	0.0731	0.000457
0.1383	0.1382	0.000503
0.3104	0.3102	0.000621
0.4099	0.4096	0.000687
0.5074	0.5070	0.000755
0.7341	0.7334	0.000914
0.8623	0.8614	0.001003
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[58]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, J. Solution Chem. **25**, 1001 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0966	0.0965	0.000620
0.1766	0.1765	0.000661
0.3597	0.3594	0.000751
0.4778	0.4774	0.000812
0.5507	0.5502	0.000845
0.7705	0.7698	0.000973
0.8708	0.8699	0.001026
1.0000	0.9989	0.001097

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[59]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-methyl-1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0668	0.0668	0.000453
0.1363	0.1362	0.000495
0.2887	0.2885	0.000586
0.3788	0.3786	0.000634
0.4842	0.4839	0.000691
0.7035	0.7029	0.000811
0.8473	0.8466	0.000876
1.0000	0.9990	0.000966

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[59]J. R. Powell, K. A. Fletcher, K. S. Coym, W. E. Acree, V. G. Varanasi, and S. W. Campbell, Int. J. Thermophys. **18**, 1495 (1997).
Variables: *T*/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-methyl-1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0844	0.0843	0.000614
0.1590	0.1589	0.000643
0.3299	0.3297	0.000706
0.4255	0.4252	0.000743
0.5327	0.5323	0.000786
0.7529	0.7522	0.000872
0.8739	0.8731	0.000914
1.0000	0.9990	0.000966

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.

(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.

(3) 99%, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

8.4. Anthracene solubility data in binary secondary alcohol + secondary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[60]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0812	0.0812	0.000445
0.1532	0.1531	0.000476
0.3184	0.3182	0.000538
0.4117	0.4115	0.000586
0.5097	0.5094	0.000610
0.7304	0.7299	0.000692
0.8564	0.8558	0.000739
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

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

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99+%, Acros Organics, USA.

Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[60]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0983	0.0982	0.000601
0.1738	0.1737	0.000618
0.3568	0.3566	0.000650
0.4481	0.4478	0.000677
0.5592	0.5589	0.000699
0.7635	0.7629	0.000741
0.8817	0.8810	0.000769
1.0000	0.9992	0.000800

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[60]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0727	0.0727	0.000440
0.1381	0.1380	0.000460
0.2927	0.2926	0.000512
0.3827	0.3825	0.000542
0.4856	0.4853	0.000578
0.7048	0.7043	0.000659
0.8458	0.8452	0.000710
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[60]J. R. Powell, M. E. R. McHale, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 728 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 4-methyl-2-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0776	0.0776	0.000601
0.1529	0.1528	0.000616
0.3215	0.3213	0.000649
0.4234	0.4232	0.000669
0.5267	0.5263	0.000689
0.7373	0.7368	0.000733
0.8539	0.8533	0.000755
1.0000	0.9992	0.000779

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

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

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99+%, Acros Organics, USA.

Components 2 and 3 were stored over anhydrous sodium sulfate and molecular sieves, and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.3% (relative error).

9. Solubility of Anthracene in Binary Alcohol + Alkoxyalcohol Solvent Mixtures

9.1. Critical evaluation of experimental solubility data

Acree and co-workers[61–66] reported the solubility of anthracene in several binary alcohol + 2-methoxyethanol, alcohol + 2-ethoxyethanol, alcohol + 2-propoxyethanol, alcohol + 2-isopropoxyethanol, alcohol + 2-butoxyethanol, and alcohol + 3-methoxy-1-butanol solvent mixtures at 298.15 K. The alcohol solvents included seven primary alcohols (1-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 3-methyl-1-butanol, 1-octanol, and 2-ethyl-1-hexanol) and four secondary alcohols (2-propanol, 2-butanol, 2-pentanol, 4-methyl-2-pentanol). There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 32 binary alcohol + alkoxyalcohol solvent systems studied are summarized in Table 8, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 8 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.1% to 0.8%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental anthracene solubility data for binary alcohol + 2-methoxyethanol alcohol + 2-ethoxyethanol,

Table 8. Mathematical representation of anthracene solubilities in binary alcohol (2) + alkoxyalcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
1-Propanol (2) + 2-methoxyethanol (3)	0.900 0.343	0.4
2-Propanol (2) + 2-methoxyethanol (3)	1.218 0.584 0.216	0.6
1-Butanol (2) + 2-methoxyethanol (3)	0.855 0.220	0.2
2-Butanol (2) + 2-methoxyethanol (3)	1.148 0.401	0.7
2-Methyl-1-propanol (2) + 2-methoxyethanol (3)	1.115 0.313	0.5
3-Methyl-1-butanol (2) + 2-methoxyethanol (3)	0.872 0.092	0.2
1-Octanol (2) + 2-methoxyethanol (3)	1.114 −0.417	0.8
1-Propanol (2) + 2-propoxyethanol (3)	0.952 0.294 0.309	0.1
2-Propanol (2) + 2-propoxyethanol (3)	1.419 0.477 0.201	0.1
1-Butanol (2) + 2-propoxyethanol (3)	0.715 0.154 0.166	0.3
2-Butanol (2) + 2-propoxyethanol (3)	1.098 0.364 0.125	0.2
1-Pentanol (2) + 2-propoxyethanol (3)	0.478 0.157 0.205	0.2
3-Methyl-1-butanol (2) + 2-propoxyethanol (3)	0.689 0.152 0.246	0.3
1-Octanol (2) + 2-propoxyethanol (3)	0.296 −0.020 0.952	0.6
1-Propanol (2) + 2-butoxyethanol (3)	1.222 0.572 0.255	0.3
2-Propanol (2) + 2-butoxyethanol (3)	1.550 0.790 0.726	0.6
1-Butanol (2) + 2-butoxyethanol (3)	0.800 0.319 0.185	0.5
2-Butanol (2) + 2-butoxyethanol (3)	1.155 0.609 0.267	0.3
2-Methyl-1-propanol (2) + 2-butoxyethanol (3)	1.292 0.606 0.316	0.2
1-Pentanol (2) + 2-butoxyethanol (3)	0.561 0.233	0.1
3-Methyl-1-butanol (2) + 2-butoxyethanol (3)	0.742 0.346 0.177	0.3
1-Octanol (2) + 2-butoxyethanol (3)	0.231 0.075 0.065	0.1
1-Propanol (2) + 3-methoxy-1-butanol (3)	0.973 0.344	0.2
2-Propanol (2) + 3-methoxy-1-butanol (3)	1.405 0.669 0.533	0.8

TABLE 8. Mathematical representation of anthracene solubilities in binary alcohol (2) + alkoxyalcohol (3) solvent mixtures—Continued

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
1-Butanol (2) + 3-methoxy-1-butanol (3)	0.667	0.3
	0.284	
2-Butanol (2) + 3-methoxy-1-butanol (3)	0.929	0.4
	0.444	
1-Pentanol (2) + 3-methoxy-1-butanol (3)	0.600	0.5
	0.222	
	0.118	
2-Pentanol (2) + 3-methoxy-1-butanol (3)	0.818	0.2
	0.161	
	0.079	
3-Methyl-1-butanol (2) + 3-methoxy-1-butanol (3)	0.766	0.6
	0.253	
4-Methyl-2-pentanol (2) + 3-methoxy-1-butanol (3)	0.644	0.4
1-Octanol (2) + 3-methoxy-1-butanol (3)	0.475	0.4
2-Ethyl-1-hexanol (2) + 3-methoxy-1-butanol (3)	0.423	0.2
	−0.167	
	−0.069	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only a single coefficient is listed, then $S_{23,1}$ and $S_{23,2}$ are zero. Similarly, if two coefficients are listed, then $S_{23,2}$ is zero.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

alcohol + 2-propoxyethanol, alcohol + 2-isopropoxyethanol, alcohol + 2-butoxyethanol, and alcohol + 3-methoxy-1-butanol solvent mixtures are given in Secs. 9.2–9.7.

9.2. Anthracene solubility data in binary alcohol + 2-methoxyethanol solvent mixtures

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[61] M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0985	0.0984	0.000746
0.1861	0.1859	0.000894
0.3889	0.3884	0.001243
0.4840	0.4833	0.001398
0.5889	0.5880	0.001571
0.7854	0.7839	0.001894
0.8953	0.8935	0.002035
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[61] M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.1037	0.1036	0.000580
0.2019	0.2017	0.000753
0.3955	0.3951	0.001090
0.4859	0.4853	0.001264
0.6006	0.5997	0.001482
0.7591	0.7577	0.001780
0.8893	0.8875	0.001996
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]
(3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]

Original Measurements:
[61]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1173	0.1172	0.001006
0.2273	0.2270	0.001192
0.4382	0.4375	0.001552
0.5362	0.5352	0.001698
0.6222	0.6211	0.001817
0.8196	0.8179	0.002052
0.9074	0.9055	0.002129
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, HPLC grade, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]
(3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]

Original Measurements:
[61]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1204	0.1203	0.000801
0.2189	0.2187	0.000978
0.4246	0.4240	0.001397
0.5376	0.5367	0.001590
0.6403	0.6392	0.001758
0.8182	0.8166	0.001969
0.9086	0.9067	0.002092
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]
(3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]

Original Measurements:
[61]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1205	0.1204	0.000657
0.2244	0.2242	0.000828
0.4402	0.4397	0.001222
0.5355	0.5347	0.001410
0.6459	0.6448	0.001627
0.8173	0.8158	0.001906
0.9128	0.9109	0.002071
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.1305	0.1303	0.001346
0.2569	0.2565	0.001544
0.4776	0.4767	0.001875
0.5784	0.5772	0.002029
0.6716	0.6702	0.002131
0.8481	0.8463	0.002179
0.9137	0.9117	0.002194
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[61]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1382	0.1381	0.000949
0.2633	0.2630	0.001159
0.4744	0.4737	0.001537
0.5845	0.5835	0.001720
0.6789	0.6776	0.001855
0.8462	0.8444	0.002075
0.9151	0.9131	0.002137
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[61]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 105 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1760	0.1756	0.002476
0.3382	0.3373	0.002711
0.5699	0.5683	0.002892
0.6651	0.6632	0.002849
0.7498	0.7477	0.002782
0.8853	0.8830	0.002562
0.9444	0.9421	0.002401
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

9.3. Anthracene solubility data in binary alcohol + 2-ethoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0759	0.0758	0.000730
0.1665	0.1663	0.000910
0.3100	0.3096	0.001217
0.4383	0.4376	0.001517
0.5398	0.5388	0.001776
0.7523	0.7506	0.002325
0.8762	0.8739	0.002675
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0887	0.0887	0.000557
0.1707	0.1706	0.000718
0.3354	0.3350	0.001078
0.4666	0.4659	0.001401
0.5441	0.5432	0.001621
0.7602	0.7585	0.002243
0.8625	0.8603	0.002555
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1028	0.1027	0.000988
0.1888	0.1886	0.001159
0.3848	0.3842	0.001563
0.4888	0.4879	0.001761
0.5921	0.5909	0.002043
0.7784	0.7765	0.002496
0.8914	0.8889	0.002785
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0995	0.0994	0.000773
0.1923	0.1921	0.000962
0.3716	0.3711	0.001375
0.4891	0.4884	0.001517
0.5959	0.5949	0.001670
0.7937	0.7921	0.001953
0.8993	0.8971	0.002467
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1023	0.1022	0.000646
0.1964	0.1962	0.000823
0.3875	0.3870	0.001250
0.4872	0.4865	0.001498
0.5876	0.5866	0.001768
0.7877	0.7858	0.002367
0.9029	0.9004	0.002745
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.1171	0.1169	0.001301
0.2231	0.2228	0.001515
0.4225	0.4217	0.001897
0.5271	0.5260	0.002097
0.6347	0.6332	0.002297
0.8113	0.8091	0.002656
0.9042	0.9016	0.002839
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1182	0.1181	0.000932
0.2204	0.2201	0.001136
0.4138	0.4131	0.001584
0.5310	0.5300	0.001853
0.6269	0.6256	0.002086
0.8172	0.8151	0.002562
0.9023	0.8998	0.002751
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[62]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and P. L. Huyskens, J. Solution Chem. **25**, 1089 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1725	0.1721	0.002502
0.2809	0.2801	0.002695
0.4978	0.4964	0.002903
0.6210	0.6191	0.003015
0.7115	0.7093	0.003085
0.8642	0.8615	0.003131
0.9291	0.9262	0.003102
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

9.4. Anthracene solubility data in binary alcohol + 2-propoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0709	0.0708	0.000735
0.1486	0.1485	0.000900
0.3066	0.3062	0.001276
0.3965	0.3959	0.001502
0.4950	0.4941	0.001770
0.7276	0.7258	0.002482
0.8745	0.8719	0.002971
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0696	0.0696	0.000541
0.1504	0.1503	0.000712
0.3099	0.3096	0.001115
0.3980	0.3975	0.001365
0.5071	0.6062	0.001696
0.7321	0.7303	0.002430
0.8729	0.8704	0.002918
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0829	0.0828	0.000969
0.1666	0.1664	0.001153
0.3408	0.3403	0.001549
0.4386	0.4378	0.001805
0.5458	0.5447	0.002078
0.7610	0.7590	0.002678
0.8717	0.8691	0.003012
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) HPLC grade, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0903	0.0902	0.000775
0.1743	0.1741	0.000963
0.3419	0.3414	0.001398
0.4364	0.4357	0.001659
0.5489	0.5478	0.001990
0.7613	0.7593	0.002617
0.8726	0.8700	0.002956
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0777	0.0777	0.000616
0.1731	0.1730	0.000813
0.3021	0.3018	0.001123
0.4566	0.4559	0.001543
0.5514	0.5504	0.001815
0.7619	0.7600	0.002516
0.8920	0.8893	0.003027
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.1038	0.1037	0.001320
0.1988	0.1985	0.001511
0.3924	0.3916	0.001930
0.4867	0.4857	0.002133
0.5881	0.5867	0.002352
0.7874	0.7852	0.002849
0.8883	0.8856	0.003095
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1006	0.1005	0.000927
0.2008	0.2006	0.001130
0.3876	0.3870	0.001560
0.4876	0.4867	0.001828
0.5879	0.5867	0.002092
0.7922	0.7900	0.002735
0.9069	0.9041	0.003080
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[63]M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **41**, 272 (1996).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1317	0.1314	0.002510
0.2656	0.2649	0.002651
0.4758	0.4744	0.002885
0.5803	0.5785	0.003039
0.6722	0.6701	0.003168
0.8438	0.8409	0.003406
0.9220	0.9188	0.003487
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

9.5. Anthracene solubility data in binary alcohol + 2-isopropoxyethanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0825	0.0824	0.000739
0.1426	0.1425	0.000856
0.3014	0.3010	0.001190
0.3913	0.3908	0.001401
0.5016	0.5008	0.001684
0.7069	0.7053	0.002229
0.8564	0.8542	0.002595
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0720	0.0720	0.000542
0.1441	0.1440	0.000683
0.3008	0.3005	0.001029
0.3990	0.3985	0.001276
0.4866	0.4859	0.001504
0.7178	0.7162	0.002175
0.8512	0.8490	0.002550
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0871	0.0870	0.000985
0.1739	0.1737	0.001147
0.3397	0.3392	0.001498
0.4222	0.4215	0.001687
0.5397	0.5386	0.001964
0.7714	0.7694	0.002580
0.8913	0.8887	0.002878
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0903	0.0902	0.000759
0.1634	0.1633	0.000903
0.3412	0.3408	0.001313
0.4474	0.4467	0.001574
0.4873	0.4865	0.001669
0.7570	0.7551	0.002378
0.8622	0.8599	0.002655
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]
(3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]

Original Measurements:

[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.0891	0.0890	0.001283
0.1956	0.1953	0.001458
0.3904	0.3897	0.001836
0.4832	0.4822	0.002006
0.5774	0.5761	0.002220
0.7838	0.6817	0.002655
0.8851	0.8826	0.002875
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]
(3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]

Original Measurements:

[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-pentanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000800
0.1088	0.1087	0.001033
0.1839	0.1837	0.001184
0.3794	0.3788	0.001590
0.4744	0.4735	0.001807
0.5883	0.5870	0.002056
0.7790	0.7770	0.002521
0.8806	0.8782	0.002740
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, Acros Organics.
(3) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]

Original Measurements:

[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1000	0.0999	0.000911
0.1948	0.1946	0.001094
0.3847	0.3841	0.001480
0.4836	0.4828	0.001703
0.5827	0.5816	0.001953
0.7856	0.7837	0.002442
0.8927	0.8903	0.002753
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]
(3) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]

Original Measurements:

[64]M. E. R. McHale, K. S. Coym, L. E. Roy, C. E. Hernández, and W. E. Acree, Jr., Can. J. Chem. **75**, 1403 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-isopropoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1495	0.1491	0.002391
0.2593	0.2586	0.002536
04700	0.4687	0.002762
0.5790	0.5773	0.002860
0.6758	0.6738	0.002990
0.8584	0.8557	0.003088
0.9123	0.9095	0.003111
1.0000	0.9969	0.003093

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99.9+%, Acros Organics, USA, was recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

9.6. Anthracene solubility data in binary alcohol + 2-butoxyethanol solvent mixtures

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Propanol; C_3H_8O; [71-23-8]
(3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]

Original Measurements:
[65]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0617	0.0616	0.000742
0.1239	0.1238	0.000900
0.2652	0.2649	0.001311
0.3642	0.3636	0.001596
0.4704	0.4695	0.001948
0.6914	0.6896	0.002667
0.8286	0.8260	0.003151
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Propanol; C_3H_8O; [67-63-0]
(3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]

Original Measurements:
[65]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0651	0.0651	0.000566
0.1286	0.1285	0.000717
0.2839	0.2836	0.001162
0.3707	0.3702	0.001434
0.4685	0.4677	0.001739
0.7016	0.6998	0.002600
0.8331	0.8305	0.003142
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[65]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0713	0.0712	0.000972
0.1401	0.1399	0.001136
0.3125	0.3120	0.001580
0.3993	0.3986	0.001834
0.5233	0.5221	0.002217
0.7119	0.7099	0.002873
0.8588	0.8560	0.003286
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[65]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0781	0.0780	0.000776
0.1526	0.1525	0.000963
0.3167	0.3162	0.001435
0.4148	0.4141	0.001738
0.5203	0.5192	0.002044
0.7364	0.7340	0.003263
0.8689	0.8661	0.003151
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[65]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0710	0.0710	0.000624
0.1520	0.1519	0.000820
0.3059	0.3055	0.001246
0.4072	0.4066	0.001539
0.5171	0.5161	0.001901
0.7352	0.7332	0.002695
0.8683	0.8655	0.003227
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[65]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.0891	0.0890	0.001302
0.1582	0.1580	0.001468
0.3558	0.3551	0.001966
0.4573	0.4563	0.002230
0.5288	0.5275	0.002420
0.7610	0.7587	0.003054
0.8791	0.8761	0.003400
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[65]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. 28, 209 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0859	0.0858	0.000918
0.2374	0.2371	0.001274
0.3557	0.3551	0.001592
0.4512	0.4504	0.001870
0.5509	0.5497	0.002141
0.7650	0.7628	0.002871
0.8719	0.8691	0.003267
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[65]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 209 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 2-butoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1249	0.1246	0.002403
0.2353	0.2347	0.002590
0.4495	0.4482	0.002950
0.5522	0.5505	0.003105
0.6430	0.6409	0.003266
0.8222	0.8193	0.003534
0.9107	0.9074	0.003661
1.0000	0.9962	0.003785

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

9.7. Anthracene solubility data in binary alcohol + 3-methoxy-1-butanol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0756	0.0755	0.000724
0.1453	0.1452	0.000859
0.3091	0.3087	0.001200
0.3996	0.3990	0.001389
0.4442	0.4435	0.001483
0.7246	0.7231	0.002092
0.8576	0.8556	0.002382
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0792	0.0792	0.000570
0.1492	0.1491	0.000705
0.3079	0.3076	0.001053
0.3921	0.3916	0.001258
0.5119	0.5111	0.001529
0.7182	0.7167	0.002059
0.8687	0.8666	0.002408
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0869	0.0868	0.000955
0.1708	0.1706	0.001113
0.3534	0.3529	0.001474
0.4257	0.4250	0.001596
0.5384	0.5374	0.001806
0.7641	0.7624	0.002220
0.8660	0.8639	0.002424
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0900	0.0899	0.000748
0.1763	0.1761	0.000912
0.3518	0.3514	0.001276
0.4653	0.4646	0.001503
0.5787	0.5777	0.001745
0.7583	0.7567	0.002143
0.8621	0.8601	0.002345
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]
(3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]

Original Measurements:

[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.1027	0.1026	0.001300
0.1966	0.1963	0.001484
0.4260	0.4252	0.001896
0.4935	0.4925	0.001980
0.5946	0.5933	0.002135
0.8129	0.8109	0.002471
0.8835	0.8812	0.002560
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]
(3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]

Original Measurements:

[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-pentanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000800
0.1016	0.1015	0.000992
0.1998	0.1996	0.001184
0.3826	0.3820	0.001567
0.4891	0.4882	0.001778
0.5970	0.5958	0.001999
0.7902	0.7883	0.002373
0.8873	0.8851	0.002533
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99%, Across Organics, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1066	0.1065	0.000920
0.1951	0.1949	0.001083
0.3847	0.3841	0.001456
0.4925	0.4917	0.001669
0.5973	0.5962	0.001890
0.7843	0.7425	0.002281
0.8828	0.8806	0.002454
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 4-methyl-2-pentanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000779
0.1207	0.1206	0.000970
0.2089	0.2087	0.001124
0.4263	0.4256	0.001537
0.5282	0.5273	0.001775
0.6035	0.6023	0.001937
0.8069	0.8050	0.002335
0.9032	0.9009	0.002531
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, Acros, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-octanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.0756	0.0754	0.002400
0.1453	0.1449	0.002518
0.3091	0.3083	0.002692
0.3996	0.3986	0.002747
0.4442	0.4430	0.002786
0.7246	0.7226	0.002779
0.8576	0.8552	0.002749
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[66]M. E. R. McHale, A.-S. M. Kauppila, S. A. Padilla, A. L. Trufant, N. U. De La Sancha, E. Velo, J. R. Powell, and W. E. Acree, Jr., J. Chem. Eng. Data **42**, 54 (1997).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-ethyl-1-hexanol + 3-methoxy-1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001397
0.1432	0.1430	0.001586
0.2603	0.2598	0.001770
0.4770	0.4760	0.002118
0.5773	0.5760	0.002283
0.6751	0.6735	0.002414
0.8432	0.8410	0.002611
0.9231	0.9206	0.002662
1.0000	0.9973	0.002702

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

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:

(1) 99.9%, Acros Organics, USA, recrystallized several times from acetone.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99+%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

10. Solubility of Anthracene in Binary Alcohol + Ester Solvent Mixtures

10.1. Critical evaluation of experimental solubility data

Acree and co-workers[67–71] measured the solubility of anthracene in binary alcohol + methyl ethanoate, alcohol + ethyl ethanoate, alcohol + propyl ethanoate, and alcohol + butyl ethanoate solvent mixtures at 298.15 K. The alcohol solvents included five primary alcohols (1-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 3-methyl-1-butanol) and three secondary alcohols (2-propanol, 2-butanol, 2-pentanol). There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 25 binary alcohol + alkyl ethanoate solvent systems studied are summarized in Table 9, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 9 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 1.0%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

Jouyban and co-workers[68] employed a molarity form of the Combined NIBS/Redlich-Kister equation

$$\ln x_1^{\text{sat}} = x_2^{(s)} \ln (c_1^{\text{sat}})_2 + x_3^{(s)} \ln (c_1^{\text{sat}})_3 + x_2^{(s)} x_3^{(s)} \sum_{j}^{r} S_{23,j} (x_2^{(s)} - x_3^{(s)})^j \tag{14}$$

in reporting the solubility of anthracene in binary and ternary mixtures of cyclohexanone, ethyl ethanoate, and methanol at 298.2 K. Solubilities are often expressed in the pharmaceutical industry as molar concentrations (mol dm^{-3}). The derived mathematical expression

$$\ln x_1^{\text{sat}} = x_2^{(s)} \ln 0.006 + x_3^{(s)} \ln 0.049 + x_2^{(s)} x_3^{(s)} \left[2.907 + 1.990 \left(x_2^{(s)} - x_3^{(s)}\right) + 1.591 \left(x_2^{(s)} - x_3^{(s)}\right)^2\right] \tag{15}$$

was found to describe the observed anthracene solubility data for the binary methanol + ethyl ethanoate system to within an overall average relative deviation of 3.5%.

The experimental anthracene solubility data for binary alcohol + methyl ethanoate solvent mixtures, for binary alcohol + ethyl ethanoate, for binary alcohol + propyl ethanoate, and for binary alcohol + butyl ethanoate solvent mixtures are given in Secs. 10.2–10.5.

Table 9. Mathematical representation of anthracene solubilities in binary alcohol (2) + alkyl ethanoate (3) solvent mixtures

Binary Solvent System	$S_{23,i}$[a]	% Dev[b]
1-Propanol (2) + methyl ethanoate (3)	1.939	0.6
	0.691	
	0.453	
2-Propanol (2) + methyl ethanoate (3)	2.177	0.7
	0.947	
	0.418	
1-Butanol (2) + methyl ethanoate (3)	1.673	0.3
	0.328	
	0.230	
2-Butanol (2) + methyl ethanoate (3)	2.106	0.5
	0.744	
	0.564	
2-Methyl-1-propanol (2) + methyl ethanoate (3)	2.211	0.4
	0.714	
	0.587	
1-Pentanol (2) + methyl ethanoate (3)	1.775	0.6
	0.330	
	0.120	
2-Pentanol (2) + methyl ethanoate (3)	1.916	0.4
	0.558	
	0.375	
3-Methyl-1-butanol (2) + methyl ethanoate (3)	1.915	0.3
	0.417	
	−0.076	
1-Propanol (2) + ethyl ethanoate (3)	1.837	0.5
	0.828	
	0.572	
2-Propanol (2) + ethyl ethanoate (3)	2.085	0.9
	1.162	
	0.900	
1-Butanol (2) + ethyl ethanoate (3)	1.634	0.7
	0.686	
	0.041	
2-Butanol (2) + ethyl ethanoate (3)	1.987	0.2
	0.945	
	0.341	
2-Methyl-1-propanol (2) + ethyl ethanoate (3)	1.914	0.5
	0.904	
	0.268	
3-Methyl-1-butanol (2) + ethyl ethanoate (3)	1.599	0.6
	0.539	
	0.272	
1-Propanol (2) + propyl ethanoate (3)	2.040	0.9
	1.110	
	0.815	
2-Propanol (2) + propyl ethanoate (3)	2.274	1.0
	1.566	
	1.132	
1-Butanol (2) + propyl ethanoate (3)	1.656	0.5
	0.706	
	0.729	
2-Butanol (2) + propyl ethanoate (3)	1.994	0.9
	1.118	
	1.026	
2-Methyl-1-propanol (2) + propyl ethanoate (3)	2.048	0.7
	1.218	
	1.187	
3-Methyl-1-butanol (2) + propyl ethanoate (3)	1.544	0.6
	0.745	
	0.705	
1-Propanol (2) + butyl ethanoate (3)	2.252	0.5
	0.947	
	0.361	

TABLE 9. Mathematical representation of anthracene solubilities in binary alcohol (2) + alkyl ethanoate (3) solvent mixtures—Continued

Binary Solvent System	$S_{23,i}$[a]	% Dev[b]
2-Propanol (2) + butyl ethanoate (3)	2.448	0.7
	1.428	
	1.319	
1-Butanol (2) + butyl ethanoate (3)	1.701	0.8
	0.697	
	0.615	
2-Butanol (2) + butyl ethanoate (3)	2.136	0.5
	1.254	
	0.725	
2-Methyl-1-propanol (2) + butyl ethanoate (3)	2.241	0.6
	1.169	
	0.753	
3-Methyl-1-butanol (2) + butyl ethanoate (3)	1.767	0.4
	0.753	
	0.398	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\text{exp}} - x_1^{\text{cal}}]/x_1^{\text{exp}}\ |$.

10.2. Anthracene solubility data in binary alcohol + methyl ethanoate solvent mixtures

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[67] W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.1001	0.1000	0.000913
0.1904	0.1904	0.001230
0.3882	0.3881	0.001946
0.4908	0.4898	0.00235
0.5952	0.5936	0.00274
0.7889	0.7863	0.00328
0.8805	0.8774	0.00349
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[67] W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.1177	0.1176	0.000735
0.1959	0.1957	0.001006
0.3782	0.3776	0.001634
0.4887	0.4877	0.00206
0.5987	0.5972	0.00247
0.7864	0.7840	0.00311
0.8821	0.8792	0.00334
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[67]W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1390	0.1388	0.001260
0.2247	0.2243	0.001571
0.4285	0.4275	0.00236
0.5350	0.5336	0.00270
0.6378	0.6359	0.00303
0.8238	0.8209	0.00350
0.9075	0.9042	0.00361
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.

(2) 99.8%, Aldrich Chemical Company.

(3) 99.5%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[67]W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1246	0.1245	0.001017
0.2150	0.2147	0.001375
0.4262	0.4253	0.00217
0.5440	0.5426	0.00264
0.6377	0.6358	0.00296
0.9088	0.9056	0.00347
0.8805	0.8773	0.00359
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99.5%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[67]W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1192	0.1191	0.000832
0.2371	0.2368	0.001249
0.4358	0.4349	0.00203
0.5342	0.5329	0.00239
0.6429	0.6411	0.00283
0.8241	0.8213	0.00341
0.9120	0.9087	0.00357
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]
(3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]

Original Measurements:
[67]W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.1302	0.1300	0.001630
0.2612	0.2606	0.00217
0.4757	0.4743	0.00301
0.5814	0.6794	0.00337
0.6673	0.6649	0.00357
0.8454	0.8422	0.00374
0.9195	0.9161	0.00370
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 2-Pentanol; $C_5H_{12}O$; [6032-27-7]
(3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]

Original Measurements:
[67]W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-pentanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000800
0.1349	0.1347	0.001320
0.2576	0.2571	0.001821
0.4706	0.4694	0.00262
0.5936	0.5918	0.00308
0.6746	0.6724	0.00329
0.8480	0.8449	0.00361
0.9202	0.9168	0.00365
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, Acros Organics, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[67]W. E. Acree, Jr., J. Chem. Eng. Data **46**, 885 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + methyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1474	0.1472	0.001214
0.2682	0.2678	0.001677
0.4899	0.4886	0.00260
0.5722	0.5706	0.00287
0.6787	0.6765	0.00319
0.8531	0.8501	0.00350
0.9412	0.9378	0.00360
1.0000	0.9964	0.00364

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

10.3. Anthracene solubility data in binary alcohol + ethyl ethanoate solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methanol; CH_4O; [67-56-1] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[68]A. Jouyban, J. L. Manzoori, V. Panahi-Azar, J. Soleymani, M. A. A. Fakhree, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 2607 (2010).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	c_1
0.000	0.006
0.044	0.013
0.093	0.016
0.149	0.022
0.215	0.034
0.291	0.039
0.381	0.056
0.489	0.068
0.621	0.095
0.787	0.111
1.000	0.136

[a] $x_3^{(s)}$: initial mole fraction of component 3 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99.5%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:

Temperature: ±0.2 K.
$x_3^{(s)}$: ±0.005.
c_1: ±0.2% to ±5.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[69]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 327 (2002).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0813	0.0812	0.000874
0.1607	0.1605	0.001185
0.3340	0.3334	0.001936
0.4303	0.4293	0.002337
0.5441	0.5425	0.002886
0.7484	0.7455	0.003870
0.8557	0.8520	0.004293
1.0000	0.9952	0.004842

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

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[69]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 327 (2002).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.1024	0.1023	0.000742
0.1756	0.1754	0.000994
0.3478	0.3472	0.001691
0.4462	0.4452	0.002149
0.5394	0.5380	0.002554
0.7502	0.7474	0.003669
0.8694	0.8657	0.004250
1.0000	0.9952	0.004842

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

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[69]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 327 (2002).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1045	0.1044	0.001191
0.1874	0.1871	0.001537
0.3802	0.3793	0.002389
0.4713	0.4700	0.002804
0.5821	0.5802	0.003325
0.7878	0.7846	0.004097
0.8820	0.8781	0.004391
1.0000	0.9952	0.004842

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[69]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 327 (2002).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1022	0.1021	0.000950
0.1966	0.1963	0.001362
0.3851	0.3842	0.002238
0.4869	0.4856	0.002698
0.5851	0.5833	0.003137
0.7876	0.7844	0.004013
0.8867	0.8828	0.004414
1.0000	0.9952	0.004842

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[69]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 327 (2002).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0978	0.0977	0.000757
0.1920	0.1918	0.001099
0.3787	0.3780	0.001863
0.4926	0.4914	0.002397
0.5773	0.5757	0.002801
0.7953	0.7826	0.003823
0.8959	0.8920	0.004310
1.0000	0.9952	0.004842

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[69]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **40**, 327 (2002).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + ethyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1184	0.1183	0.001145
0.2225	0.2222	0.001554
0.4240	0.4230	0.002424
0.5238	0.5223	0.002913
0.6244	0.6223	0.003392
0.8130	0.8096	0.004205
0.9022	0.8981	0.004512
1.0000	0.9952	0.004842

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

10.4. Anthracene solubility data in binary alcohol + propyl ethanoate solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[70]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + propyl ethanoate mixtures[a]

$x_3^{(s)\ b}$	x_3	x_1
0.0000	0.0000	0.000591
0.0781	0.0780	0.000917
0.1415	0.1413	0.001211
0.3048	0.3042	0.00205
0.3895	0.3885	0.00252
0.5022	0.5006	0.00309
0.7187	0.7156	0.00438
0.8397	0.8355	0.00504
1.0000	0.9941	0.00588

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

[b] There was a typographical error in the solvent compositions reported. The authors inadvertently gave identical values for both 1-propanol + propyl ethanoate and 1-butanol + propyl ethanoate. The values in the table above are correct.

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[70]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: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + propyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0714	0.0714	0.000672
0.1352	0.1351	0.000931
0.3510	0.3503	0.001973
0.4018	0.4009	0.00225
0.5016	0.5002	0.00280
0.7254	0.7224	0.00410
0.8374	0.8334	0.00479
1.0000	0.9941	0.00588

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[70]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: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + propyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0872	0.0871	0.001189
0.1634	0.1631	0.001548
0.3403	0.3395	0.00241
0.4416	0.4403	0.00297
0.5377	0.5358	0.00352
0.7587	0.7551	0.00478
0.8699	0.8652	0.00538
1.0000	0.9941	0.00588

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, recrystallized several times from acetone.
(2) 99%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[70]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: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + propyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0842	0.0841	0.000946
0.1636	0.1634	0.001311
0.3427	0.3419	0.00221
0.4310	0.4298	0.00269
0.5447	0.5429	0.00335
0.7581	0.7546	0.00464
0.8632	0.8587	0.00523
1.0000	0.9941	0.00588

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[70]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + propyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0853	0.0852	0.000791
0.1755	0.1753	0.001185
0.3477	0.3470	0.001987
0.4462	0.4451	0.00248
0.5508	0.5491	0.00309
0.7562	0.7529	0.00441
0.8650	0.8606	0.00513
1.0000	0.9941	0.00588

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[70]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + propyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0890	0.0889	0.001085
0.1932	0.1929	0.001552
0.3811	0.3802	0.00242
0.4848	0.4834	0.00294
0.5842	0.5821	0.00354
0.7905	0.7867	0.00478
0.8877	0.8830	0.00532
1.0000	0.9941	0.00588

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, recrystallized several times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

10.5. Anthracene solubility data in binary alcohol + butyl ethanoate solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[71]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 773 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + butyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.0674	0.0673	0.000859
0.1322	0.1320	0.001160
0.2774	0.2768	0.002034
0.3649	0.3640	0.002571
0.4605	0.4590	0.003169
0.6933	0.6900	0.004776
0.8347	0.8300	0.005667
1.0000	0.9934	0.006611

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.7%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[71]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 773 (2001).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + butyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.0608	0.0608	0.000639
0.1249	0.1248	0.000923
0.2709	0.2704	0.001685
0.3676	0.3668	0.002252
0.4734	0.4720	0.002900
0.6928	0.6897	0.004474
0.8278	0.8233	0.005471
1.0000	0.9934	0.006611

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.7%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[71]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 773 (2001).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + butyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.0741	0.0740	0.001131
0.1497	0.1495	0.001513
0.3023	0.3016	0.002329
0.4077	0.4065	0.002926
0.5098	0.5080	0.003618
0.7328	0.7290	0.005125
0.8464	0.8415	0.005782
1.0000	0.9934	0.006611

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99.7%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[71]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 773 (2001).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + butyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.0750	0.0749	0.000909
0.1523	0.1521	0.001308
0.3160	0.3153	0.002239
0.4090	0.4079	0.002780
0.5120	0.5102	0.003470
0.7299	0.7264	0.004802
0.8547	0.8498	0.005675
1.0000	0.9934	0.006611

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.7%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[71]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 773 (2001).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + butyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.0811	0.0810	0.000773
0.1451	0.1449	0.001052
0.3134	0.3128	0.001950
0.4138	0.4128	0.002535
0.5139	0.5123	0.003193
0.6937	0.6906	0.004459
0.8466	0.8419	0.005536
1.0000	0.9934	0.006611

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company.
(3) 99.7%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[71]A. Toro and W. E. Acree, Jr., Phys. Chem. Liq. **39**, 773 (2001).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-methyl-1-butanol + butyl ethanoate mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.0878	0.0877	0.001089
0.1724	0.1721	0.001517
0.3487	0.3478	0.002481
0.4532	0.4518	0.003103
0.5276	0.5257	0.003581
0.7573	0.7534	0.005112
0.8716	0.8665	0.005831
1.0000	0.9934	0.006611

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.7%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

11. Solubility of Anthracene in Binary Alcohol + Alkanenitrile Solvent Mixtures

11.1. Critical evaluation of experimental solubility data

Acree and co-workers[72,73] determined the solubility of anthracene in 13 binary solvent mixtures containing acetonitrile with methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 2-methyl-1-pentanol, and 4-methyl-2-pentanol at 298.15 K. There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 13 binary alcohol + acetonitrile solvent systems studied are summarized in Table 10, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 10 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.4% to 1.0%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

TABLE 10. Mathematical representation of anthracene solubilities in binary alcohol (2) + acetonitrile (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Methanol (2) + acetonitrile (3)	1.170	0.5
	0.514	
	0.189	
Ethanol (2) + acetonitrile (3)	1.722	0.6
	0.753	
	0.379	
1-Propanol (2) + acetonitrile (3)	2.478	0.7
	0.042	
	1.200	
2-Propanol (2) + acetonitrile (3)	2.736	0.5
	0.827	
	0.968	
1-Butanol (2) + acetonitrile (3)	2.986	0.4
	−0.033	
	0.952	
2-Butanol (2) + acetonitrile (3)	3.323	0.5
	0.529	
	1.031	
2-Methyl-1-propanol (2) + acetonitrile (3)	3.256	0.5
	0.549	
	1.232	
1-Pentanol (2) + acetonitrile (3)	3.164	0.6
	−0.545	
	0.956	
2-Pentanol (2) + acetonitrile (3)	3.449	0.6
	−0.265	
	1.659	
3-Methyl-1-butanol (2) + acetonitrile (3)	2.963	0.4
	−0.365	
	0.952	
2-Methyl-1-butanol (2) + acetonitrile (3)	3.116	0.6
	−0.528	
	0.687	
2-Methyl-1-pentanol (2) + acetonitrile (3)	3.529	0.9
	−0.727	
	1.074	
4-Methyl-2-pentanol (2) + acetonitrile (3)	3.262	1.0
	−0.622	
	1.825	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\mathrm{exp}} - x_1^{\mathrm{cal}}]/x_1^{\mathrm{exp}}\ |$.

The experimental anthracene solubility data for binary alcohol + acetonitrile solvent mixtures are given in Sec. 11.2.

11.2. Anthracene solubility data in binary alcohol + acetonitrile solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methanol; CH_4O; [67-56-1] (3) Acetonitrile; C_2H_3N; [75-05-8]	[72] C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 720 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000243
0.0979	0.0979	0.000320
0.1674	0.1673	0.000370
0.3437	0.3435	0.000502
0.4429	0.4429	0.000565
0.5419	0.5416	0.000627
0.7414	0.7409	0.000735
0.8667	0.8660	0.000778
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.

(2) 99.9+%, Aldrich Chemical Company.

(3) 99.8%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Ethanol; C_2H_6O; [64-17-5] (3) Acetonitrile; C_2H_3N; [75-05-8]	[72] C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 720 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in ethanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000460
0.1363	0.1362	0.000669
0.2231	0.2229	0.000773
0.4283	0.4279	0.000917
0.5316	0.5311	0.000962
0.6349	0.6343	0.000961
0.8175	0.8167	0.000924
0.9030	0.9022	0.000880
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) absolute, Asper Alcohol and Chemical Company, USA.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000591
0.1466	0.1465	0.000910
0.2683	0.2680	0.001128
0.4747	0.4741	0.001305
0.5662	0.5655	0.001318
0.6824	0.6815	0.001291
0.8491	0.8481	0.001168
0.9293	0.9283	0.001109
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.1799	0.1798	0.000806
0.2814	0.2811	0.000958
0.5049	0.5043	0.001163
0.5969	0.5962	0.001182
0.6600	0.6592	0.001162
0.8555	0.8546	0.001036
0.9224	0.9215	0.000956
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1850	0.1848	0.001339
0.3224	0.3219	0.001581
0.5377	0.5368	0.001712
0.6384	0.6373	0.001677
0.7171	0.7160	0.001564
0.8729	0.8718	0.001227
0.9308	0.9298	0.001064
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99.8+%, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1679	0.1677	0.001108
0.3044	0.3040	0.001409
0.5297	0.5289	0.001593
0.6076	0.6066	0.001588
0.7303	0.7292	0.001451
0.8692	0.8682	0.001174
0.9359	0.9349	0.001101
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 356 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-propanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000470
0.1671	0.1669	0.000925
0.3175	0.3171	0.001223
0.5276	0.5268	0.001440
0.6351	0.6342	0.001401
0.7258	0.7248	0.001361
0.8715	0.8705	0.001145
0.9339	0.9330	0.001005
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0] (3) Acetonitrile; C_2H_3N; [75-05-8]	[72]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 720 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-pentanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001097
0.2022	0.2019	0.001723
0.3421	0.3414	0.002021
0.5734	0.5722	0.002066
0.6662	0.6649	0.001971
0.7555	0.7542	0.001750
0.8886	0.8875	0.001288
0.9443	0.9433	0.001065
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7] (3) Acetonitrile; C_2H_3N; [75-05-8]	[72]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 720 (2003).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-pentanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000800
0.1955	0.1952	0.001484
0.3448	0.3442	0.001807
0.5837	0.5826	0.001947
0.6773	0.6760	0.001867
0.7165	0.7152	0.001792
0.8879	0.8867	0.001300
0.9426	0.9416	0.001090
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, Acros Organics, USA.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 3-methyl-1-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000727
0.1843	0.1841	0.001186
0.3445	0.3440	0.001489
0.5738	0.5728	0.001658
0.6751	0.6740	0.001595
0.7384	0.7373	0.001526
0.8884	0.8873	0.001197
0.9482	0.9471	0.001108
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (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] (3) Acetonitrile; C_2H_3N; [75-05-8]	[73]K. M. De Fina, S. Abernathy, K. Alexander, C. Olugbuyi, A. Vance, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 402 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000786
0.1908	0.1906	0.001277
0.3468	0.3463	0.001577
0.5779	0.5769	0.001755
0.6724	0.6712	0.001729
0.7534	0.7522	0.001597
0.8864	0.8853	0.001232
0.9434	0.9424	0.001028
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99+%, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (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] (3) Acetonitrile; C_2H_3N; [75-05-8]	[72] C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 720 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-methyl-1-pentanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000966
0.2110	0.2107	0.001653
0.3755	0.3747	0.002064
0.6179	0.6166	0.002109
0.7071	0.7057	0.001972
0.7780	0.7766	0.001816
0.9008	0.8996	0.001291
0.9435	0.9425	0.001095
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99.9+%, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (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] (3) Acetonitrile; C_2H_3N; [75-05-8]	[72] C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 720 (2003).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 4-methyl-2-pentanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000779
0.2136	0.2133	0.001407
0.3425	0.3419	0.001679
0.6078	0.6067	0.001881
0.6793	0.6781	0.001817
0.7897	0.7884	0.001631
0.9028	0.9017	0.001265
0.9523	0.9513	0.001059
1.0000	0.9992	0.000830

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from acetone.
(2) 99.9+%, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.0% (relative error).

TABLE 11. Mathematical representation of anthracene solubilities in binary alkoxyalcohol (2) + alkoxyalcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
2-Ethoxyethanol (2) + 2-methoxyethanol (3)	0.185	0.2
	0.116	
2-Propoxyethanol (2) + 2-methoxyethanol (3)	0.361	0.3
2-Butoxyethanol (2) + 2-methoxyethanol (3)	0.515	0.4
2-Propoxyethanol (2) + 2-ethoxyethanol (3)	0.122	0.2
	−0.089	
	0.306	
2-Butoxyethanol (2) + 2-ethoxyethanol (3)	0.327	0.5
2-Butoxyethanol (2) + 2-propoxyethanol (3)	0.111	0.2

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only a single coefficient is listed, then $S_{23,1}$ and $S_{23,2}$ are zero. Similarly, if two coefficients are listed, then $S_{23,2}$ is zero.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\text{exp}} - x_1^{\text{cal}}]/x_1^{\text{exp}}\ |$.

12. Solubility of Anthracene in Binary Alkoxyalcohol + Alkoxyalcohol Solvent Mixtures

12.1. Critical evaluation of experimental solubility data

McHale *et al.*[74] determined the solubility of anthracene in binary 2-ethoxyethanol + 2-methoxyethanol, 2-propoxyethanol + 2-methoxyethanol, 2-butoxyethanol + 2-methoxyethanol, 2-propoxyethanol + 2-ethoxyethanol, 2-butoxyethanol + 2-ethoxyethanol and 2-butoxyethanol + 2-propoxyethanol solvent mixtures at 298.15 K. There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the six binary alkoxyalcohol + alkoxyalcohol solvent systems studied are summarized in Table 11, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 11 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.2% to 0.5%, indicating that the measured values fall on smooth $\ln x_1$ versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental anthracene solubility data for binary alkoxyalcohol + alkoxyalcohol solvent mixtures are listed in Sec. 12.2.

12.2. Anthracene solubility data in binary alkoxyalcohol + alkoxyalcohol solvent mixtures

Components:	Original Measurements:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[74] M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 589 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-ethoxyethanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002921
0.1278	0.1274	0.002912
0.2399	0.2392	0.002855
0.4193	0.4182	0.002724
0.5530	0.5516	0.002602
0.6435	0.6419	0.002524
0.8294	0.8274	0.002360
0.9089	0.9068	0.002286
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Acros Organics, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[74]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 589 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propoxyethanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.003343
0.1438	0.1433	0.003307
0.2675	0.2666	0.003217
0.4897	0.4882	0.002978
0.5937	0.5920	0.002870
0.6888	0.6869	0.002715
0.8322	0.8301	0.002487
0.9271	0.9249	0.002330
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[74]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 589 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butoxyethanol + 2-methoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.003785
0.1522	0.1516	0.003712
0.2993	0.2982	0.003564
0.5147	0.5130	0.003245
0.6212	0.6193	0.003060
0.7149	0.7128	0.002883
0.8576	0.8554	0.002554
0.9433	0.9411	0.002345
1.0000	0.9978	0.002211

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Acros Organics, USA.
(3) 99.5%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[74]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 589 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propoxyethanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.003343
0.1214	0.1210	0.003373
0.2314	0.2306	0.003328
0.4382	0.4368	0.003241
0.5204	0.5187	0.003214
0.6383	0.6366	0.003206
0.8191	0.8165	0.003118
0.9088	0.9060	0.003060
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[74]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 589 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butoxyethanol + 2-ethoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.003785
0.1441	0.1436	0.003808
0.2516	0.2506	0.003777
0.4727	0.4710	0.003601
0.5748	0.5728	0.003518
0.6701	0.6678	0.003405
0.8387	0.8360	0.003201
0.9185	0.9157	0.003073
1.0000	0.9971	0.002921

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

(1) 99.9+%, Gold Label, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) 99%, Acros Organics, USA.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
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] (3) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[74]M. E. R. McHale, A.-S. M. Kauppila, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **28**, 589 (1996).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-butoxyethanol + 2-propoxyethanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.003785
0.1103	0.1099	0.003778
0.2279	0.2270	0.003743
0.4345	0.4329	0.003690
0.5325	0.5306	0.003619
0.6371	0.6348	0.003572
0.8228	0.8199	0.003479
0.9163	0.9131	0.003509
1.0000	0.9967	0.003343

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

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Source and Purity of Chemicals:

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

(2) 99%, Acros Organics, USA.

(3) 99%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

13. Solubility of Anthracene in Miscellaneous Binary Solvent Mixtures

13.1. Critical evaluation of experimental solubility data

There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. In the absence of replicate independent measurements, the experimental values were evaluated by curve-fitting the measured solubility data to the molarity version of the Combined NIBS/Redlich-Kister equation [See Eq. (14)]. The calculated $S_{23,i}$ parameters for the five binary ketone + alcohol and one ketone + alkyl ethanoate solvent systems studied are summarized in Table 12, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 12 reveals that Eq. (14) does provide a very accurate mathematical representation for how the measured molar solubilities vary with binary solvent composition. Average percent deviations range from 1.5% to 6.2%, indicating that the measured values fall on smooth ln c_1 versus $x_2^{(s)}$ curves. Experimental uncertainties associated with the molar solubility data ranged from 0.2% to 5.0 percent relative deviation. None of the experimental data points was flagged as an outlier.

The experimental anthracene solubility data for binary alcohol + propanone, methanol + cyclohexanone, and cyclohexanone + ethyl ethanoate solvent mixtures are given in Secs. 13.2 and 13.3.

TABLE 12. Mathematical representation of anthracene solubilities in miscellaneous binary solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Methanol (2) + propanone (3)	2.320	2.4
	0.989	
	0.449	
Ethanol (2) + propanone (3)	1.791	3.7
	0.114	
	0.617	
	2.677	
1-Propanol (2) + propanone (3)	2.205	1.5
	1.387	
	−0.474	
2-Propanol (2) + propanone (3)	1.314	2.6
	0.566	
	−0.310	
Cyclohexanone (2) + methanol (3)	3.601	6.2
	−2.715	
	3.790	
Cyclohexanone (2) + ethyl ethanoate (3)	0.835	2.8
	−1.041	
	1.209	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, $S_{23,2}$, and $S_{23,3}$. If only three coefficients are listed, then $S_{23,3}$ is zero.

[b] Dev (%) = (100/N) Σ | [$c_1^{\text{exp}} - c_1^{\text{cal}}$]/$c_1^{\text{exp}}$ |.

13.2. Anthracene solubility data in binary ketone + alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methanol; CH_4O; [67-56-1] (3) Propanone; C_3H_6O; [67-64-1]	[75] A. Jouyban, J. L. Manzoori, J. Soleymani, V. Panahi-Azar, M. A. A. Fakhree, S. Ahmadian, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 5319 (2010).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in methanol + propanone mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.0527
0.168	0.0470
0.312	0.0427
0.437	0.0374
0.547	0.0308
0.644	0.0233
0.731	0.0196
0.809	0.0153
0.879	0.0112
0.942	0.0088
1.000	0.0063

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99%, Scharlan Chemie, Spain, no further purification specified.
(3) 99.5%, Scharlan Chemie, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±2.4% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Ethanol; C_2H_6O; [64-17-4]
(3) Propanone; C_3H_6O; [67-64-1]

Original Measurements:
[75]A. Jouyban, J. L. Manzoori, J. Soleymani, V. Panahi-Azar, M. A. A. Fakhree, S. Ahmadian, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 5319 (2010).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in ethanol + propanone mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.0527
0.123	0.0470
0.240	0.0432
0.351	0.0431
0.457	0.0372
0.558	0.0291
0.654	0.0246
0.746	0.0231
0.835	0.0166
0.919	0.0136
1.000	0.0087

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99.9%, Scharlan Chemie, Spain, no further purification specified.
(3) 99.5%, Scharlan Chemie, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±2.4% (relative error).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) 1-Propanol; C_3H_8O; [71-23-8]
(3) Propanone; C_3H_6O; [67-64-1]

Original Measurements:
[75]A. Jouyban, J. L. Manzoori, J. Soleymani, V. Panahi-Azar, M. A. A. Fakhree, S. Ahmadian, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 5319 (2010).

Variables:
T/K = 298.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 1-propanol + propanone mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.0527
0.098	0.0469
0.197	0.0458
0.296	0.0444
0.396	0.0413
0.496	0.0371
0.596	0.0334
0.696	0.0239
0.797	0.0198
0.898	0.0144
1.000	0.0090

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 µm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99.5%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Scharlan Chemie, no further purification specified.

Estimated Error:

Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±2.4% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Propanone; C_3H_6O; [67-64-1]	[75]A. Jouyban, J. L. Manzoori, J. Soleymani, V. Panahi-Azar, M. A. A. Fakhree, S. Ahmadian, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 5319 (2010).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in 2-propanol + propanone mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.0527
0.055	0.0474
0.116	0.0444
0.184	0.0414
0.260	0.0341
0.345	0.0307
0.441	0.0269
0.551	0.0222
0.678	0.0151
0.826	0.0105
1.000	0.0056

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 µm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99.5%, Scharlan Chemie, Spain, no further purification specified.
(3) 99.5%, Scharlan Chemie, no further purification specified.

Estimated Error:

Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±2.4% (relative error).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexanone, $C_6H_{10}O$; [108-94-1] (3) Methanol; CH_4O; [67-56-1]	[68]A. Jouyban, J. L. Manzoori, V. Panahi-Azar, J. Soleymani, M. A. A. Fakhree, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 2607 (2010).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexanone + methanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.006
0.042	0.013
0.089	0.016
0.144	0.022
0.207	0.034
0.281	0.039
0.370	0.056
0.477	0.068
0.610	0.095
0.779	0.111
1.000	0.136

[a]$x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5% Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.005.
c_1: ±0.2% to ±5.0% (relative error).

13.3. Anthracene solubility data in binary ketone + alkyl ethanoate solvent mixtures

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexanone, $C_6H_{10}O$; [108-94-1] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[68]A. Jouyban, J. L. Manzoori, V. Panahi-Azar, J. Soleymani, M. A. A. Fakhree, A. Shayanfar, and W. E. Acree, Jr., J. Chem. Eng. Data **55**, 2607 (2010).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of anthracene in cyclohexanone + ethyl ethanoate mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.049
0.096	0.074
0.193	0.078
0.290	0.085
0.389	0.094
0.489	0.103
0.589	0.107
0.690	0.114
0.793	0.124
0.896	0.125
1.000	0.136

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 96%, Fluka Chemical Company, recrystallized several times from acetone and ethyl ethanoate.
(2) 99.5%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.9%, Merck Chemical Company, Germany, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.005.
c_1: ±0.2% to ±5.0% (relative error).

14. Solubility of Naphthalene in Binary Alkane + Alcohol Solvent Mixtures

14.1. Critical evaluation of experimental solubility data

Dyshin *et al.*[76] reported the solubility of naphthalene in binary heptane + ethanol solvent mixtures at 298.15 K. Solubilities were measured at only three binary mole fraction compositions and in the two neat organic solvents. Shayanfar *et al.*[77] determined the solubility of anthracene in binary solvent mixtures containing 2,2,4-trimethylpentane with methanol, ethanol, 1-propanol, 2-propanol, and 1-butanol at 298.15 K. There has only been a single experimental determination for the solubility of naphthalene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (14).

The calculated $S_{23,i}$ parameters for the five binary alkane + alcohol solvent systems studied are summarized in Table 13, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 13 reveals that Eq. (14) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.5% to 4.6%, indicating that the measured values fall on fairly smooth $\ln x_1$ versus $x_2^{(s)}$ curves. Larger deviations between experimental and back-calculated values were noted in the binary 2,2,4-trimethylpentane + methanol system, which exhibits considerable deviations from ideality. At room temperature, 2,2,4-trimethylpentane +

TABLE 13. Mathematical representation of naphthalene solubilities in binary alkane (2) + alcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
2,2,4-Trimethylpentane (2) + methanol (3)	1.810	4.6
	0.006	
	−2.856	
	−6.442	
2,2,4-Trimethylpentane (2) + ethanol (3)	1.427	0.8
	−0.659	
	−0.210	
	0.214	
2,2,4-Trimethylpentane (2) + 1-propanol (3)	0.961	1.4
	−0.252	
	0.342	
2,2,4-Trimethylpentane (2) + 1-butanol (3)	0.827	0.5
	0.303	
	0.232	
2,2,4-Trimethylpentane (2) + 2-propanol (3)	1.002	2.5
	−0.228	
	1.257	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, $S_{23,2}$, and $S_{23,3}$. If only three coefficients are listed, then $S_{23,3}$ is zero.
[b] $\text{Dev (\%)} = (100/N)\ \Sigma\ |\ [c_1^{\text{exp}} - c_1^{\text{cal}}]/c_1^{\text{exp}}\ |$.

methanol mixtures do separate into two liquid phases at methanol mole fraction concentrations between 0.3 and 0.85 mole fraction. None of the experimental data points was flagged as an outlier.

The experimental naphthalene solubility data for binary alkane + alcohol solvent mixtures are reported in Secs. 14.2 and 14.3.

14.2. Naphthalene solubility data in binary alkane + primary alcohol solvent mixtures

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5] (3) Heptane; C_7H_{16}; [142-82-5]	[76] A. A. Dyshin, O. V. Eliseeva, M. G. Kiselev, and G. A. Al'per, Russ. J. Phys. Chem. A **82**, 1258 (2008).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of naphthalene in ethanol + heptane mixtures[a]

$x_3^{(s)}$	m_1
0.0000	0.90690
0.0200	0.92210
0.0404	0.94325
0.0600	1.15012
1.0000	1.30125

[a] $x_3^{(s)}$: initial mole fraction of component 3 in the binary solvent mixture; m_1: molality solubility of the solute in the ternary solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very few experimental details were provided. Paper states that the solutions were prepared gravimetrically and that the solubility was studied by the isothermal saturation method. Equilibrium was established in two days.

Source and Purity of Chemicals:
(1) Purity not specified, Riedle-de Haën.
(2) Purity and chemical source not specified.
(3) Chemically pure grade for chromatography, chemical source not specified.

Estimated Error:
Temperature: ±0.01 K.
$x_3^{(s)}$: ±0.0001 (compiler).
m_1: Not specified in paper.

Components:	Original Measurements:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) Methanol; CH_4O; [67-64-1]	[77] 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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of naphthalene in 2,2,4-trimethylpentane + methanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.540
0.026	0.623
0.058	0.668
0.095	0.705
0.140	0.746
0.196	0.850
0.268	0.882
0.363	0.922
0.494	0.871
0.687	0.823
1.000	0.692

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 274 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99+%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.002.
c_1: ±2.4% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) Ethanol; C_2H_6O; [64-17-5]	[77]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of naphthalene in 2,2,4-trimethylpentane + ethanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.558
0.038	0.596
0.081	0.652
0.131	0.700
0.190	0.746
0.260	0.820
0.345	0.847
0.450	0.901
0.584	0.871
0.760	0.796
1.000	0.692

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99+%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.002.
c_1: ±2.4% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1-Propanol; C_3H_8O; [71-23-8]	[77]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of naphthalene in 2,2,4-trimethylpentane + 1-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.601
0.048	0.683
0.102	0.698
0.162	0.723
0.232	0.770
0.312	0.789
0.404	0.810
0.514	0.820
0.644	0.836
0.803	0.772
1.000	0.692

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 99%, Fluka Chemical Company, was used as received.
(2) 99+%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.002.
c_1: ±2.4% (relative error).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[77]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of naphthalene in 2,2,4-trimethylpentane + 1-butanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.705
0.058	0.732
0.122	0.764
0.192	0.786
0.270	0.812
0.356	0.834
0.454	0.845
0.564	0.877
0.689	0.847
0.833	0.815
1.000	0.692

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 99%, Fluka Chemical Company, was used as received.
(2) 99+%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:

Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.002.
c_1: ±2.4% (relative error).

14.3. Naphthalene solubility data in binary alkane + secondary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 2-Propanol; C_3H_8O; [67-63-0]	[77]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of naphthalene in 2,2,4-trimethylpentane + 2-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.571
0.049	0.649
0.104	0.693
0.166	0.730
0.236	0.751
0.317	0.778
0.410	0.816
0.520	0.865
0.650	0.835
0.807	0.804
1.000	0.692

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 356 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 99%, Fluka Chemical Company, was used as received.
(2) 99+%, Merck Chemical Company, Germany, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:

Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.002.
c_1: ±2.4% (relative error).

15. Solubility of Phenanthrene in Binary Alkane + Alcohol Solvent Mixtures

15.1. Critical evaluation of experimental solubility data

Shayanfar *et al.*[39] determined the solubility of phenanthrene in binary 2,2,4-trimethylpentane + ethanol solvent mixtures at 298.15, 308.15, and 318.15 K. There has only been a single experimental determination for the solubility of phenanthrene in this binary solvent system. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (14). Analysis of the experimental solubility for phenanthrene in 2,2,4-trimethylpentane (2) + ethanol (3) yielded the following three mathematical representations:

$$\begin{aligned}\ln x_1{}^{\mathrm{sat}}\ (\mathrm{at\ 298\ K}) &= x_2{}^{(\mathrm{s})}\ln(0.0246) + x_3{}^{(\mathrm{s})}\ln(0.0119)\\ &\quad + x_2{}^{(\mathrm{s})}x_3{}^{(\mathrm{s})}\big[1.566 - 0.471\,(x_2{}^{(\mathrm{s})} - x_3{}^{(\mathrm{s})})\\ &\quad + 0.619\,(x_2{}^{(\mathrm{s})} - x_3{}^{(\mathrm{s})})^2\big], \end{aligned} \tag{16}$$

$$\begin{aligned}\ln x_1{}^{\mathrm{sat}}\ (\mathrm{at\ 308\ K}) &= x_2{}^{(\mathrm{s})}\ln(0.0378) + x_3{}^{(\mathrm{s})}\ln(0.0159)\\ &\quad + x_2{}^{(\mathrm{s})}x_3{}^{(\mathrm{s})}\big[1.694 - 0.980\,(x_2{}^{(\mathrm{s})} - x_3{}^{(\mathrm{s})})\\ &\quad + 0.367\,(x_2{}^{(\mathrm{s})} - x_3{}^{(\mathrm{s})})^2\big], \end{aligned} \tag{17}$$

$$\begin{aligned}\ln x_1{}^{\mathrm{sat}}\ (\mathrm{at\ 318\ K}) &= x_2{}^{(\mathrm{s})}\ln(0.0484) + x_3{}^{(\mathrm{s})}\ln(0.0190)\\ &\quad + x_2{}^{(\mathrm{s})}x_3{}^{(\mathrm{s})}\big[1.458 - 0.487\,(x_2{}^{(\mathrm{s})} - x_3{}^{(\mathrm{s})})\\ &\quad + 1.301\,(x_2{}^{(\mathrm{s})} - x_3{}^{(\mathrm{s})})^2\big], \end{aligned} \tag{18}$$

having average absolute relative deviations of 1.8%, 2.2%, and 1.6%, respectively. The reproducibility in the measured mole fraction solubilities was ±2.5%. The deviations between the experimental and back-calculated values based on the Combined NIBS/Redlich-Kister model do not seem unreasonable given the uncertainties associated with the observed solubility data.

15.2. Phenanthrene solubility data in binary alkane + primary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) Ethanol; C_2H_6O; [64-17-5]	[39]A. Shayanfar, S. H. Eghrary, F. Sardari, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **56**, 2290 (2011).
Variables:	**Prepared by:**
T/K = 298.2, 308.2, 318.2; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in 2,2,4-trimethylpentane + ethanol mixtures[a]

T/K	$x_3{}^{(\mathrm{s})}$	x_3	x_1
298.2	0.000	0.000	0.0246
	0.239	0.232	0.0272
	0.414	0.403	0.0266
	0.548	0.535	0.0239
	0.653	0.639	0.0220
	0.739	0.723	0.0213
	0.809	0.793	0.0196
	0.868	0.853	0.0171
	0.919	0.905	0.0149
	0.962	0.949	0.0134
	1.000	0.988	0.0119
308.2	0.000	0.000	0.0378
	0.242	0.233	0.0385
	0.418	0.402	0.0388
	0.552	0.533	0.0347
	0.657	0.636	0.0320
	0.742	0.720	0.0298
	0.812	0.790	0.0273
	0.870	0.850	0.0234
	0.920	0.900	0.0212
	0.963	0.946	0.0181
	1.000	0.984	0.0159
318.2	0.000	0.000	0.0484
	0.240	0.228	0.0510
	0.415	0.395	0.0473
	0.549	0.526	0.0421
	0.654	0.629	0.0384
	0.739	0.713	0.0358
	0.810	0.784	0.0322
	0.869	0.844	0.0282
	0.919	0.896	0.0254
	0.962	0.940	0.0227
	1.000	0.981	0.0190

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

Auxiliary Information

Method/Apparatus/Procedure:

Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with methanol. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) 98%, Merck Chemical Company, Germany, recrystallized several times from acetone.

(2) 99%, Merck Chemical Company, no further purification specified.

(3) 99.9%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_3^{(s)}$: ±0.001.
x_1: ±2.5% (relative error).

16. Solubility of Phenanthrene in Binary Alcohol + Alcohol Solvent Mixtures

16.1. Critical evaluation of experimental solubility data

Fakhree *et al.*[78,79] measured the solubility of phenanthrene in binary solvent mixtures containing two alcohol solvents. The solvents included four primary alcohols (methanol, ethanol, 1-propanol, and 1-butanol) and one secondary alcohol (2-propanol). There has only been a single experimental determination for the solubility of phenanthrene in each of the binary solvent systems studied. In the absence of replicate independent measurements, the experimental values were evaluated by curve-fitting the measured solubility data to Eq. (14). The calculated $S_{23,i}$ parameters for the ten binary alcohol + alcohol solvent systems studied are summarized in Table 14, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 14 reveals that Eq. (14) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.4% to 1.7%, indicating that the measured values fall on fairly smooth $\ln x_1$ versus $x_2^{(s)}$ curves. Computations showed that the molar solubility of naphthalene in the binary methanol + ethanol system at an ethanol mole fraction of $x_2^{(s)} = 0.862$ was likely high by about 5 or 6 relative percent, which is slightly larger than the reproducibility of 3.5% reported by Fakhree and co-workers.

The experimental phenanthrene solubility data for binary primary alcohol + primary alcohol and primary alcohol + secondary alcohol solvent mixtures are given in Secs. 16.2 and 16.3.

TABLE 14. Mathematical representation of phenanthrene solubilities in binary alcohol (2) + alcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Ethanol (2) + methanol (3)	0.450	1.5
	−0.192	
	−0.535	
Methanol (2) + 1-propanol (3)	1.079	1.5
	0.847	
	0.864	
Methanol (2) + 1-butanol (3)	1.255	0.8
	0.604	
	0.356	
Ethanol (2) + 1-propanol (3)	0.260	0.4
	−0.165	
	0.065	
Ethanol (2) + 1-butanol (3)	0.339	1.1
	0.346	
	−0.244	
1-Propanol (2) + 1-butanol (3)	−0.018	0.8
	−0.191	
	0.066	
Methanol (2) + 2-propanol (3)	0.741	1.7
	0.400	
	−0.063	
Ethanol (2) + 2-propanol (3)	0.238	1.5
	−0.141	
	0.106	
1-Propanol (2) + 2-propanol (3)	0.037	0.6
	0.156	
	−0.606	
1-Butanol (2) + 2-propanol (3)	0.116	1.5
	0.232	
	−0.263	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.
[b] Dev (%) = $(100/N)\,\Sigma\,|\,[c_1^{\text{exp}} - c_1^{\text{cal}}]/c_1^{\text{exp}}\,|$.

16.2. Phenanthrene solubility data in binary primary alcohol + primary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5] (3) Methanol; CH_4O; [67-56-1]	[78] M. A. A. Fakhree, A. Shayanfar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **54**, 1405 (2009).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in ethanol + methanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.133
0.071	0.138
0.148	0.147
0.229	0.152
0.316	0.165
0.409	0.170
0.510	0.178
0.618	0.177
0.735	0.180
0.862	0.192
1.000	0.187

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was used as received.
(2) 99.9%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±3.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Methanol; CH_4O; [67-56-1] (3) 1-Propanol; C_3H_8O; [71-23-8]	[79]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in methanol + 1-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.174
0.170	0.187
0.316	0.196
0.442	0.202
0.552	0.208
0.649	0.200
0.735	0.193
0.812	0.183
0.881	0.173
0.943	0.156
1.000	0.133

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was recrystallized several times from acetone.
(2) 99.5%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Methanol; CH_4O; [67-56-1] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[79]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in methanol + 1-butanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.194
0.201	0.213
0.361	0.216
0.492	0.219
0.601	0.217
0.693	0.207
0.772	0.198
0.841	0.181
0.900	0.163
0.953	0.149
1.000	0.133

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was recrystallized several times from acetone.
(2) 99.5%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5] (3) 1-Propanol; C_3H_8O; [71-23-8]	[79]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in ethanol + 1-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.174
0.125	0.184
0.243	0.187
0.354	0.188
0.461	0.190
0.562	0.190
0.658	0.189
0.749	0.187
0.837	0.186
0.920	0.183
1.000	0.182

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was recrystallized several times from acetone.
(2) 99.9%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[79]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in ethanol + 1-butanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.194
0.148	0.193
0.282	0.195
0.402	0.198
0.511	0.203
0.610	0.204
0.702	0.205
0.785	0.203
0.862	0.197
0.934	0.186
1.000	0.182

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was recrystallized several times from acetone.
(2) 99.9%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±4.2% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[79]M. A. A. Fakhree, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **55**, 531 (2010).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in 1-propanol + 1-butanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.194
0.120	0.194
0.234	0.193
0.344	0.190
0.449	0.188
0.550	0.182
0.647	0.177
0.741	0.172
0.830	0.171
0.917	0.175
1.000	0.174

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was recrystallized several times from acetone.
(2) 99.9%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±4.2% (relative error).

16.3. Phenanthrene solubility data in binary primary alcohol + secondary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Methanol; CH_4O; [67-56-1] (3) 2-Propanol; C_3H_8O; [67-63-0]	[78]M. A. A. Fakhree, A. Shayanfar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **54**, 1405 (2009).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in methanol + 2-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.124
0.174	0.135
0.321	0.142
0.447	0.147
0.557	0.157
0.654	0.160
0.739	0.153
0.815	0.154
0.883	0.148
0.944	0.139
1.000	0.133

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±3.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) Ethanol; C_2H_6O; [64-17-5] (3) 2-Propanol; C_3H_8O; [67-63-0]	[78]M. A. A. Fakhree, A. Shayanfar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **54**, 1405 (2009).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in ethanol + 2-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.124
0.127	0.138
0.247	0.143
0.359	0.152
0.466	0.159
0.567	0.169
0.663	0.170
0.753	0.170
0.840	0.176
0.922	0.184
1.000	0.187

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was used as received.
(2) 99.9%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±3.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Propanol; C_3H_8O; [67-63-0]	[78]M. A. A. Fakhree, A. Shayanfar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **54**, 1405 (2009).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in 1-propanol + 2-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.124
0.102	0.122
0.204	0.130
0.305	0.134
0.405	0.141
0.505	0.148
0.605	0.153
0.705	0.157
0.803	0.161
0.902	0.165
1.000	0.174

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±3.5% (relative error).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{10}H_8$; [91-20-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Propanol; C_3H_8O; [67-63-0]	[78]M. A. A. Fakhree, A. Shayanfar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **54**, 1405 (2009).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenanthrene in 1-butanol + 2-propanol mixtures[a]

$x_2^{(s)}$	c_1
0.000	0.124
0.085	0.124
0.173	0.135
0.264	0.138
0.358	0.146
0.455	0.156
0.556	0.159
0.661	0.168
0.770	0.174
0.883	0.183
1.000	0.188

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture; c_1: molar solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with propanone. Molar concentrations determined by spectrophotometric measurements at 345 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, Merck Chemical Company, no further purification specified.
(3) 99.5%, Merck Chemical Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_2^{(s)}$: ±0.001.
c_1: ±3.5% (relative error).

17. Solubility of Phenothiazine in Binary Alcohol + 1,2-Alkanediol Solvent Mixtures

17.1. Critical evaluation of experimental solubility data

Ahmadian *et al.*[80] determined the solubility of phenothiazine in binary ethanol + 1,2-propanediol (also called propylene glycol) solvent mixtures at 298.15 K. There has only been a single experimental determination for the solubility of phenothiazine in this binary solvent system. Analysis of the experimental solubility for phenothiazine dissolved in ethanol (2) + 1,2-propanediol (3) yielded the following mathematical representation:

$$\begin{aligned}\ln x_1^{\mathrm{sat}}\,(\text{at } 298\ \mathrm{K}) &= x_2^{(s)} \ln(0.008753) + x_3^{(s)} \ln(0.004226)\\ &\quad + x_2^{(s)} x_3^{(s)}\left[0.430 - 0.502\left(x_2^{(s)} - x_3^{(s)}\right)\right.\\ &\quad \left. + 0.603\left(x_2^{(s)} - x_3^{(s)}\right)^2\right] \qquad (19)\end{aligned}$$

having an average absolute relative deviation between observed and back-calculated phenothiazine solubility of 1.6%.

17.2. Phenothiazine solubility data in binary ethanol + 1,2-propanediol solvent mixtures

Components:	**Original Measurements:**
(1) Phenothiazine; $C_{12}H_9NS$; [92-84-2] (2) Ethanol; C_2H_6O; [64-17-5] (3) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[80]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:**
T/K = 298.2; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of phenothiazine in ethanol + 1,2-propanediol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.000	0.000	0.00875
0.184	0.183	0.00875
0.337	0.334	0.00888
0.465	0.461	0.00853
0.575	0.570	0.00838
0.670	0.665	0.00794
0.753	0.747	0.00747
0.826	0.820	0.00704
0.890	0.884	0.00642
0.948	0.943	0.00527
1.000	0.996	0.00423

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

Auxiliary Information

Method/Apparatus/Procedure:
Shaker bath, incubator equipped with temperature controlling system, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in sealed containers and allowed to equilibrate for three days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a hydrophobic Drapore filters (0.45 μm, Millipore, Ireland) into tared volumetric flasks, weighed and diluted with ethanol. Molar concentrations determined by spectrophotometric measurements at 317 nm. The measured molar solubilities were converted to mole fraction solubilities using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) 98%, Merck Chemical Company, Germany, recrystallized several times from acetone.
(2) 99.9%, Scharlau Chemie Company, Spain, no further purification specified.
(3) 99.5%, Scharlau Chemie Company, no further purification specified.

Estimated Error:
Temperature: ±0.2 K.
$x_3^{(s)}$: ±0.001.
x_1: ±2.7% (relative error).

18. Solubility of Pyrene in Binary Alkane + Alcohol Solvent Mixtures

18.1. Critical evaluation of experimental solubility data

Volume 59 in the IUPAC Solubility Data Series[3] contained solubility data for 14 binary solvent mixtures containing hexane, heptane, octane, cyclohexane, methylcyclohexane, and 2,2,4-trimethylpentane with 1-propanol and 2-propanol. For the most part, the solubility data were measured at 299.2 K and seven compositions spanning the entire binary mole fraction range. To conserve space, data from the earlier volume will not be repeated in this volume. Attention will be focused on compiling experimental values determined after Vol. 59 was published.

Acree and co-workers[32,81–83] measured the solubility of pyrene in several binary alkane + 1-butanol, alkane + 2-butanol, alkane + 2-methyl-1-propanol, and alkane + 1-octanol solvent mixtures at 299.15 K. The alkane solvents included hexane, heptane, octane, cyclohexane, methylcyclohexane, 2,2,4-trimethylpentane, and *tert*-butylcyclohexane (also called (1,1-dimethylethyl)cyclohexane). There has only been a single experimental determination for the solubility of pyrene in each of the binary solvent systems studied. In the absence of replicate independent measurements, the experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 25 binary alkane + alcohol solvent systems studied are summarized in Table 15, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 15 reveals that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.1% to 1.4%, indicating that the measured values fall on smooth $\ln x_1$ versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental pyrene solubility data for binary alkane + primary alcohol and binary alkane + secondary alcohol solvent mixtures are given in Secs. 18.2 and 18.3.

TABLE 15. Mathematical representation of pyrene solubilities in binary alkane (2) + alcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Hexane (2) + 1-butanol (3)	0.882	0.1
	0.299	
	0.551	
Heptane (2) + 1-butanol (3)	1.075	0.3
	0.189	
	0.388	
Octane (2) + 1-butanol (3)	1.239	0.7
	−0.039	
	0.365	
Cyclohexane (2) + 1-butanol (3)	0.976	0.6
	0.462	
	0.472	
Methylcyclohexane (2) + 1-butanol (3)	1.143	0.5
	0.269	
	0.629	
2,2,4-Trimethylpentane (2) + 1-butanol (3)	0.826	0.3
	0.105	
	0.875	
Hexane (2) + 2-butanol (3)	1.344	0.5
	−0.128	
	0.216	
Heptane (2) + 2-butanol (3)	1.583	0.5
	−0.232	
	0.392	
Octane (2) + 2-butanol (3)	1.631	0.5
	−0.490	
	0.794	
Cyclohexane (2) + 2-butanol (3)	1.426	0.5
	0.064	
	0.447	
Methylcyclohexane (2) + 2-butanol (3)	1.512	0.5
	−0.091	
	0.670	
2,2,4-Trimethylpentane (2) + 2-butanol (3)	1.148	0.7
	−0.274	
	0.558	
Hexane (2) + 2-methyl-1-propanol (3)	1.407	0.2
	0.072	
	0.211	
Heptane (2) + 2-methyl-1-propanol (3)	1.604	0.4
	−0.151	
	0.545	
Octane (2) + 2-methyl-1-propanol (3)	1.794	0.6
	−0.387	
	0.419	
Cyclohexane (2) + 2-methyl-1-propanol (3)	1.316	0.6
	0.427	
	0.190	
Methylcyclohexane (2) + 2-methyl-1-propanol (3)	1.624	0.3
	0.138	
	0.616	
2,2,4-Trimethylpentane (2) + 2-methyl-1-propanol (3)	1.605	0.3
	0.207	
	0.532	
Hexane (2) + 1-octanol (3)	0.828	1.4
	0.836	
	0.855	
Heptanol (2) + 1-octanol (3)	0.667	1.0
	0.664	
	0.574	
Octane (2) + 1-octanol (3)	0.591	1.0
	0.557	
	0.430	

18.2. Pyrene solubility data in binary alkane + primary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Hexane; C_6H_{14}; [110-54-3] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in hexane + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00857
0.1567	0.1552	0.00972
0.2639	0.2613	0.00969
0.4865	0.4821	0.00910
0.5882	0.5830	0.00876
0.6833	0.6776	0.00836
0.8509	0.8446	0.00735
0.9170	0.9107	0.00689
1.0000	0.9938	0.00622

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

TABLE 15. Mathematical representation of pyrene solubilities in binary alkane (2) + alcohol (3) solvent mixtures—Continued

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
Cyclohexane (2) + 1-octanol (3)	0.588	1.4
	0.875	
	1.011	
Methylcyclohexane (2) + 1-octanol (3)	0.463	1.3
	0.880	
	0.832	
2,2,4-Trimethylpentane (2) + 1-octanol (3)	0.704	0.8
	0.628	
	0.584	
tert-Butylcyclohexane (2) + 1-octanol (3)	0.518	0.9
	0.470	
	0.438	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\text{exp}} - x_1^{\text{cal}}]/x_1^{\text{exp}}\ |$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Heptane; C_7H_{16}; [142-82-5] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[81] T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998)
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in heptane + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01102
0.1641	0.1621	0.01210
0.2924	0.2889	0.01205
0.5148	0.5093	0.01073
0.6140	0.6079	0.00990
0.7066	0.7000	0.00920
0.8570	0.8504	0.00775
0.9358	0.9293	0.00694
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, HPLC grade, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Octane; C_8H_{18}; [111-65-9] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[81] T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in octane + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01372
0.1797	0.1794	0.01462
0.3107	0.3064	0.01397
0.5445	0.5379	0.01206
0.6422	0.6351	0.01105
0.7321	0.7247	0.01007
0.8807	0.8737	0.00798
0.9396	0.9329	0.00712
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in cyclohexane + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01100
0.1344	0.1327	0.01229
0.2319	0.2291	0.01213
0.4311	0.4263	0.01112
0.5380	0.5325	0.01030
0.6433	0.6373	0.00940
0.8226	0.8162	0.00776
0.9045	0.8981	0.00712
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99.9+%, HPLC grade, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in methylcyclohexane + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01292
0.1542	0.1520	0.01434
0.2634	0.2597	0.01389
0.4752	0.4694	0.01219
0.5829	0.5765	0.01106
0.6717	0.6649	0.01011
0.8451	0.8381	0.00831
0.9194	0.9127	0.00726
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[32]E. M. Debase and W. E. Acree, Jr., J. Chem. Eng. Data **46**, 1464 (2001).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2,2,4-trimethylpentane + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00720
0.2001	0.1984	0.00848
0.3122	0.3095	0.00849
0.5407	0.5363	0.00817
0.6409	0.6357	0.00806
0.7307	0.7250	0.00779
0.8832	0.8769	0.00716
0.9334	0.9270	0.00687
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8%, anhydrous, Aldrich Chemical Company.
(3) 99.8+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in hexane + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00857
0.1458	0.1445	0.00907
0.2706	0.2682	0.00878
0.4827	0.4790	0.00764
0.5899	0.5859	0.00682
0.6823	0.6782	0.00603
0.8488	0.8449	0.00455
0.9270	0.9234	0.00387
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in heptane + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01102
0.1679	0.1660	0.01146
0.2885	0.2854	0.01078
0.5141	0.5095	0.00886
0.6110	0.6062	0.00781
0.7071	0.7024	0.00666
0.8500	0.8457	0.00502
0.9221	0.9182	0.00418
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Octane; C_8H_{18}; [111-65-9] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in octane + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01372
0.1796	0.1794	0.01373
0.3174	0.3135	0.01244
0.5436	0.5383	0.00984
0.6357	0.6302	0.00858
0.7122	0.7068	0.00758
0.8774	0.8730	0.00501
0.9473	0.9435	0.00397
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in cyclohexane + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01100
0.1365	0.1349	0.01149
0.2315	0.2290	0.01092
0.4339	0.4300	0.00904
0.5428	0.5385	0.00783
0.6534	0.6491	0.00660
0.8253	0.8214	0.00476
0.9057	0.9021	0.00400
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99.9+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[81]T. L. Borders, M. E. McHale, J. R. Powell, K. S. Coym, C. E. Hernández, L. E. Roy, W. E. Acree, Jr., D. C. Williams, and S. W. Campbell, Fluid Phase Equilib. **146**, 207 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in methylcyclohexane + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01292
0.1423	0.1404	0.01365
0.2639	0.2605	0.01272
0.4723	0.4675	0.01016
0.5618	0.5568	0.00892
0.6799	0.6750	0.00725
0.8433	0.8390	0.00513
0.9285	0.9247	0.00410
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Hexane; C_6H_{14}; [110-54-3] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in hexane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00857
0.0942	0.0931	0.01131
0.1759	0.1768	0.01262
0.3561	0.3508	0.01499
0.4589	0.4515	0.01615
0.5504	0.5410	0.01705
0.7636	0.7490	0.01917
0.8707	0.8535	0.01978
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Heptane; C_7H_{16}; [142-82-5] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in heptane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01102
0.1106	0.1091	0.01386
0.1922	0.1893	0.01492
0.3794	0.3720	0.01693
0.4800	0.4714	0.01782
0.5842	0.5733	0.01868
0.7886	0.7730	0.01979
0.8724	0.8548	0.02017
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Octane; C_8H_{18}; [111-65-9] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in octane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01372
0.1181	0.1161	0.01659
0.2157	0.2119	0.01760
0.4040	0.3963	0.01904
0.5097	0.4997	0.01971
0.6084	0.5962	0.02013
0.7991	0.7827	0.02051
0.8975	0.8790	0.02061
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99.9+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in cyclohexane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01100
0.0810	0.0799	0.01364
0.1510	0.1488	0.01479
0.3125	0.3073	0.01654
0.4070	0.3999	0.01733
0.5121	0.5029	0.01788
0.7291	0.7151	0.01917
0.8399	0.8233	0.01976
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]
(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in methylcyclohexane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01292
0.0905	0.0891	0.01576
0.1698	0.1669	0.01681
0.3534	0.3470	0.01800
0.4523	0.4439	0.01851
0.5581	0.5476	0.01881
0.7524	0.7377	0.01951
0.8627	0.8455	0.01990
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99.9+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2,2,4-trimethylpentane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00720
0.1126	0.1116	0.00953
0.2175	0.2151	0.01102
0.4160	0.4104	0.01357
0.5153	0.5077	0.01483
0.6128	0.6030	0.01606
0.8053	0.7904	0.01846
0.8853	0.8681	0.01940
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) *tert*-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[82]A. I. Zvaigzne and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1127 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in *tert*-butylcyclohexane + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01594
0.1171	0.1149	0.01865
0.2223	0.2180	0.01940
0.4201	0.4115	0.02050
0.5237	0.5127	0.02096
0.6298	0.6166	0.02102
0.8086	0.7917	0.02095
0.8985	0.8796	0.02098
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from methanol.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

18.3. Pyrene solubility data in binary alkane + secondary alcohol solvent mixtures

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Hexane; C_6H_{14}; [110-54-3] (3) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[83]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **30**, 37 (1998).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in hexane + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00857
0.1521	0.1507	0.00926
0.2621	0.2597	0.00917
0.4836	0.4794	0.00866
0.5879	0.5832	0.00807
0.6827	0.6776	0.00741
0.8564	0.8514	0.00581
0.9242	0.9194	0.00517
1.0000	0.9956	0.00439

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from methanol.
(2) 99%, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Heptane; C_7H_{16}; [142-82-5] (3) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[83]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **30**, 37 (1998).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in heptane + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01102
0.1581	0.1562	0.01182
0.2941	0.2907	0.01155
0.5030	0.4978	0.01040
0.6129	0.6072	0.00927
0.7066	0.7007	0.00828
0.8666	0.8612	0.00618
0.9289	0.9239	0.00539
1.0000	0.9956	0.00439

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from methanol.
(2) 99%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) Octane; C_8H_{18}; [111-65-9] (3) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[83]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **30**, 37 (1998).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in octane + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01372
0.1847	0.1821	0.01427
0.3137	0.3095	0.01333
0.5238	0.5178	0.01138
0.6383	0.6318	0.01011
0.7295	0.7229	0.00902
0.8739	0.8681	0.00658
0.9304	0.9251	0.00565
1.0000	0.9956	0.00439

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
[83]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **30**, 37 (1998).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in cyclohexane + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01100
0.1319	0.1303	0.01192
0.2322	0.2295	0.01166
0.4374	0.4328	0.01047
0.5375	0.5323	0.00962
0.6457	0.6402	0.00851
0.8213	0.8160	0.00649
0.9199	0.9149	0.00547
1.0000	0.9956	0.00439

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from methanol.
(2) 99.9%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]
(3) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
[83]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **30**, 37 (1998).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in methylcyclohexane + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.01292
0.1522	0.1501	0.01382
0.2648	0.2613	0.01318
0.4810	0.4756	0.01128
0.5809	0.5750	0.01010
0.6842	0.6783	0.00879
0.8456	0.8400	0.00659
0.9171	0.9119	0.00563
1.0000	0.9956	0.00439

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from methanol.
(2) 99%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(3) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
[83]C. E. Hernández, K. S. Coym, L. E. Roy, J. R. Powell, and W. E. Acree, Jr., J. Chem. Thermodyn. **30**, 37 (1998).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2,2,4-trimethylpentane + 2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00720
0.1802	0.1788	0.00783
0.3285	0.3259	0.00791
0.5401	0.5361	0.00743
0.6430	0.6385	0.00697
0.7299	0.7251	0.00658
0.8800	0.8751	0.00553
0.9388	0.9341	0.00504
1.0000	0.9956	0.00439

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized three times from methanol.

(2) 99.7%, HPLC grade, Aldrich Chemical Company.

(3) 99+%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

19. Solubility of Pyrene in Binary Alcohol + Alcohol Solvent Mixtures

19.1. Critical evaluation of experimental solubility data

Acree and co-workers[84–88] reported the solubility of pyrene in several binary alcohol + alcohol solvent systems at 299.15 K. The solvents included seven primary alcohols (1-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 3-methyl-1-butanol, 1-octanol, and 2-ethyl-1-hexanol), four secondary alcohols (2-propanol, 2-butanol, 4-methyl-2-pentanol, and cyclohexanol), and one tertiary alcohol (2-methyl-2-propanol). There has only been a single experimental determination for the solubility of pyrene in each of the binary solvent systems studied. In the absence of replicate independent measurements, the experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the 44 binary alcohol + alcohol solvent systems studied are summarized in Table 16, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Curve-fit parameters were not required to describe the observed solubility behavior pyrene in several of the binary solvent systems (e.g., 1-butanol + 2-methyl-2-butanol, 3-methyl-1-butanol + 2-methyl-2-butanol, 2-butanol + 1-propanol, 2-methyl-1-propanol + 1-propanol). Examination of the numerical entries in the last column of Table 16 reveals that Eq. (10)

TABLE 16. Mathematical representation of pyrene solubilities in binary alcohol (2) + alcohol (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
2-Butanol (3) + 1-butanol (3)	0.007 −0.011 0.326	0.3
1-Butanol (3) + 1-octanol (3)	0.676 0.314 0.221	0.2
2-Butanol (2) + 1-octanol (3)	0.891 0.519 0.143	0.4
2-Butanol (2) + 2-methyl-1-propanol (3)	0.052 0.092 0.206	0.1
3-Methyl-1-butanol (2) + 1-butanol (3)	0.003 0.085 0.171	0.3
3-Methyl-1-butanol (2) + 2-methyl-1-propanol (3)	0.259 0.072 0.206	0.5
1-Propanol (2) + cyclohexanol (3)	0.340 0.104 0.153	0.5
2-Propanol (2) + cyclohexanol (3)	0.489 0.139 0.178	0.8
1-Butanol (2) + cyclohexanol (3)	0.176 0.053	0.3
2-Butanol (2) + cyclohexanol (3)	0.284 0.100 0.277	0.4
2-Methyl-1-propanol (2) + cyclohexanol (3)	0.191 0.128 0.114	0.6
1-Propanol (2) + 1-pentanol (3)	0.309 0.074 −0.205	0.4
2-Propanol (2) + 1-pentanol (3)	0.510 0.012	0.6
1-Butanol (2) + 1-pentanol (3)	0.148 −0.042 0.157	0.4
2-Butanol (2) + 1-pentanol (3)	0.144	0.5
2-Methyl-1-propanol (2) + 1-pentanol (3)	0.359 0.077	0.4
2-Pentanol (2) + 1-pentanol (3)	0.062 0.000 0.131	0.4

TABLE 16. Mathematical representation of pyrene solubilities in binary alcohol (2) + alcohol (3) solvent mixtures—Continued

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
3-Methyl-1-butanol (2) + 1-pentanol (3)	0.074	0.2
	0.024	
1-Propanol (2) + 2-methyl-2-butanol (3)	−0.079	0.4
2-Propanol (2) + 2-methyl-2-butanol (3)	0.131	0.3
	0.019	
	−0.069	
1-Butanol (2) + 2-methyl-2-butanol (3)	0.000	0.3
2-Methyl-1-propanol (2) + 2-methyl-2-butanol (3)	−0.026	0.5
	−0.073	
	−0.056	
1-Pentanol (2) + 2-methyl-2-butanol (3)	0.115	0.4
	0.058	
	0.145	
2-Pentanol (2) + 2-methyl-2-butanol (3)	−0.013	0.1
3-Methyl-1-butanol (2) + 2-methyl-2-butanol (3)	0.000	0.4
4-Methyl-2-pentanol (2) + 2-methyl-2-butanol (3)	0.062	0.2
2-Propanol (2) + 1-propanol (3)	0.036	0.5
1-Butanol (2) + 1-propanol (3)	0.127	0.4
	0.065	
2-Butanol (2) + 1-propanol (3)	0.000	0.5
2-Methyl-1-propanol (2) + 1-propanol (3)	0.000	0.8
3-Methyl-1-butanol (2) + 1-propanol (3)	0.081	0.2
	0.061	
1-Octanol (2) + 1-propanol (3)	1.153	0.3
	−0.562	
	0.685	
1-Butanol (2) + 2-propanol (3)	0.215	0.5
2-Butanol (2) + 2-propanol (3)	0.270	0.3
2-Methyl-1-propanol (2) + 2-propanol (3)	0.185	0.4
3-Methyl-1-butanol (2) + 2-propanol (3)	0.190	0.2
	0.089	
1-Octanol (2) + 2-propanol (3)	1.450	1.3
	−0.882	
	1.076	
1-Propanol (2) + 2-ethyl-1-hexanol (3)	0.500	0.5
	0.300	
2-Propanol (2) + 2-ethyl-1-hexanol (3)	0.696	0.3
	0.573	
	0.274	
1-Butanol (2) + 2-ethyl-1-hexanol (3)	0.048	0.4
	0.152	
	0.291	
2-Butanol (2) + 2-ethyl-1-hexanol (3)	0.486	0.3
2-Methyl-1-propanol (2) + 2-ethyl-1-hexanol (3)	0.594	0.6
	0.405	
3-Methyl-1-butanol (2) + 2-ethyl-1-hexanol (3)	0.024	0.4
	0.139	
	0.252	
1-Octanol (2) + 2-ethyl-1-hexanol (3)	−0.094	0.3

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$. If only a single coefficient is listed, then $S_{23,1}$ and $S_{23,2}$ are zero. Similarly, if two coefficients are listed, then $S_{23,2}$ is zero.

[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\text{exp}} - x_1^{\text{cal}}]/x_1^{\text{exp}}\ |$.

does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.1% to 1.3%, indicating that the measured values fall on smooth $\ln x_1$ versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

Solubility data are arranged according to alcohol type. The experimental pyrene solubility data for binary primary alcohol + primary, primary alcohol + secondary alcohol primary alcohol + tertiary alcohol, secondary alcohol + secondary alcohol, secondary alcohol + tertiary alcohol solvent mixtures are given in Secs. 19.2–19.6.

19.2. Anthracene solubility data in binary primary alcohol + primary alcohol solvent

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[84] M. E. R. McHale, A. I. Zvaigzne, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, Phys. Chem. Liq. **32**, 67 (1996).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.0642	0.0637	0.00720
0.1279	0.1269	0.00810
0.2677	0.2650	0.01022
0.3731	0.3687	0.01168
0.4687	0.4626	0.01303
0.7018	0.6903	0.01640
0.8546	0.8386	0.01870
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

Original Measurements:
[84]M. E. R. McHale, A. I. Zvaigzne, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, Phys. Chem. Liq. **32**, 67 (1996).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1214	0.1207	0.00538
0.2251	0.2239	0.00514
0.4337	0.4317	0.00471
0.5369	0.5345	0.00443
0.6371	0.6345	0.00415
0.8236	0.8205	0.00371
0.9121	0.9089	0.00351
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
[84]M. E. R. McHale, A. I. Zvaigzne, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, Phys. Chem. Liq. **32**, 67 (1996).

Variables:
T/K = 299.15; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1164	0.1157	0.00565
0.2450	0.2436	0.00570
0.4335	0.4310	0.00581
0.5414	0.5382	0.00586
0.6364	0.6326	0.00596
0.8240	0.8190	0.00606
0.9063	0.9007	0.00618
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8+%, HPLC grade, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 1-Propanol; C_3H_8O; [71-23-8]
(3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]

Original Measurements:
[85]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-propanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00426
0.0739	0.0736	0.00457
0.1553	0.2545	0.00501
0.3232	0.3213	0.00589
0.4146	0.4120	0.00634
0.5181	0.5145	0.00688
0.7356	0.7298	0.00788
0.8568	0.8495	0.00850
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 1-Propanol; C_3H_8O; [71-23-8]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + 1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.1265	0.1257	0.00606
0.2295	0.2282	0.00587
0.4508	0.4484	0.00543
0.5503	0.5475	0.00515
0.6450	0.6418	0.00496
0.8337	0.8299	0.00460
0.9162	0.9121	0.00443
1.0000	0.9957	0.00426

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 1-Propanol; C_3H_8O; [71-23-8]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-methyl-1-propanol + 1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.1281	0.1277	0.00341
0.2296	0.2288	0.00348
0.4522	0.4505	0.00366
0.5446	0.5426	0.00375
0.6510	0.6485	0.00385
0.8251	0.8218	0.00401
0.9171	0.9133	0.00414
1.0000	0.9957	0.00426

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 1-Propanol; C_3H_8O; [71-23-8]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables: *T*/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1508	0.1500	0.00535
0.2637	0.2623	0.00522
0.5110	0.5085	0.00493
0.6012	0.5983	0.00481
0.6886	0.6854	0.00469
0.8444	0.8406	0.00448
0.9269	0.9228	0.00437
1.0000	0.9957	0.00426

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

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(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 1-Propanol; C_3H_8O; [71-23-8]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables: *T*/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-octanol + 1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.02077
0.2155	0.2117	0.01782
0.3558	0.3505	0.01504
0.5782	0.5716	0.01138
0.6799	0.6733	0.00968
0.7663	0.7600	0.00824
0.8895	0.8840	0.00616
0.9439	0.9390	0.00524
1.0000	0.9957	0.00426

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]
(3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]

Original Measurements:
[85]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.0947	0.0941	0.00658
0.1709	0.1697	0.00684
0.3564	0.3537	0.00745
0.4593	0.4557	0.00781
0.5516	0.5472	0.00805
0.7672	0.7605	0.00872
0.8643	0.8564	0.00913
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-23-1]
(3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]

Original Measurements:
[85]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-methyl-1-propanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.0967	0.0963	0.00375
0.1811	0.1803	0.00419
0.3614	0.3595	0.00515
0.4621	0.4594	0.00581
0.5705	0.5668	0.00644
0.7689	0.7629	0.00779
0.8820	0.8745	0.00847
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]

Original Measurements:
[85]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; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1136	0.1129	0.00585
0.2091	0.2078	0.00621
0.4025	0.3997	0.00690
0.5031	0.4995	0.00717
0.6019	0.5973	0.00765
0.7931	0.7864	0.00839
0.8892	0.8813	0.00884
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-propanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00426
0.0573	0.0570	0.00473
0.1103	0.1097	0.00517
0.2400	0.2385	0.00618
0.3210	0.3188	0.00684
0.4405	0.4371	0.00774
0.6606	0.6544	0.00946
0.8155	0.8067	0.01081
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.0656	0.0652	0.00668
0.1314	0.1305	0.00707
0.2770	0.2749	0.00776
0.3609	0.3579	0.00818
0.4703	0.4662	0.00881
0.6889	0.6819	0.01021
0.8218	0.8127	0.01111
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.

(2) 99.8%, HPLC grade, Aldrich Chemical Company.

(3) 99+%, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-propanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.0639	0.0637	0.00376
0.1292	0.1286	0.00433
0.2622	0.2608	0.00537
0.3592	0.3570	0.00615
0.4824	0.4789	0.00722
0.7042	0.6977	0.00920
0.8052	0.8415	0.01022
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99+%, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.0765	0.0760	0.00597
0.1506	0.1496	0.00634
0.3152	0.3129	0.00722
0.4104	0.4072	0.00780
0.5090	0.5047	0.00841
0.7344	0.7270	0.01009
0.8285	0.8195	0.01088
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-octanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.02077
0.0991	0.0972	0.01965
0.2050	0.2012	0.01850
0.4039	0.3972	0.01649
0.5023	0.4944	0.01577
0.6056	0.5966	0.01483
0.7955	0.7846	0.01365
0.8911	0.8795	0.01306
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

19.3. Pyrene solubility data in binary primary alcohol + secondary alcohol solvent

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 1-Propanol; C_3H_8O; [71-23-8]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-propanol + 1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00290
0.1113	0.1110	0.00306
0.2138	0.2131	0.00317
0.4118	0.4104	0.00340
0.5035	0.5017	0.00355
0.6029	0.6007	0.00367
0.7979	0.7947	0.00395
0.8974	0.8937	0.00416
1.0000	0.9957	0.00426

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1-Propanol; C_3H_8O; [71-23-8]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.1202	0.1197	0.00438
0.2429	0.2418	0.00433
0.4566	0.4546	0.00430
0.5510	0.5486	0.00427
0.6530	0.6502	0.00427
0.8275	0.8239	0.00428
0.9105	0.9066	0.00426
1.0000	0.9957	0.00426

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Propanol; C_3H_8O; [67-63-0]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.1320	0.1312	0.00581
0.2301	0.2288	0.00545
0.4486	0.4465	0.00467
0.5611	0.5587	0.00424
0.6423	0.6397	0.00398
0.8276	0.8248	0.00339
0.9133	0.9104	0.00315
1.0000	0.9971	0.00290

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Propanol; C_3H_8O; [67-63-0]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-methyl-1-propanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.1397	0.1392	0.00330
0.2361	0.2353	0.00328
0.4363	0.4349	0.00323
0.5441	0.5424	0.00318
0.6428	0.6408	0.00312
0.8276	0.8251	0.00303
0.9084	0.9057	0.00299
1.0000	0.9971	0.00290

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Propanol; C_3H_8O; [67-63-0]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1376	0.1369	0.00516
0.2738	0.2725	0.00479
0.4880	0.4859	0.00422
0.5862	0.5839	0.00394
0.6818	0.6793	0.00368
0.8539	0.8511	0.00323
0.9218	0.9190	0.00307
1.0000	0.9971	0.00290

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Propanol; C_3H_8O; [67-63-0]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-octanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.02077
0.2046	0.2043	0.01696
0.3515	0.3465	0.01427
0.5724	0.5666	0.01011
0.6743	0.6687	0.00828
0.7599	0.7547	0.00681
0.8875	0.8833	0.00474
0.9347	0.9311	0.00384
1.0000	0.9971	0.00290

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components: (1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	**Original Measurements:** [84]M. E. R. McHale. A. I. Zvaigzne, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, Phys. Chem. Liq. **32**, 67 (1996).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 1-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.1065	0.1060	0.00465
0.1954	0.1945	0.00477
0.3926	0.3906	0.00506
0.5033	0.5006	0.00527
0.6060	0.6026	0.00546
0.7875	0.7829	0.00588
0.8789	0.8735	0.00611
1.0000	0.9938	0.00622

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99.8+%, HPLC grade, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

Components: (1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	**Original Measurements:** [84]M. E. R. McHale. A. I. Zvaigzne, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, Phys. Chem. Liq. **32**, 67 (1996).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 2-methyl-1-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.1070	0.1065	0.00436
0.1997	0.1989	0.00425
0.3971	0.3955	0.00397
0.5005	0.4986	0.00384
0.6037	0.6015	0.00371
0.7974	0.7946	0.00350
0.8933	0.8903	0.00340
1.0000	0.9967	0.00326

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.

(2) 99+%, anhydrous, Aldrich Chemical Company.

(3) 99+%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.05 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

Components: (1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 1-Octanol; $C_8H_{18}O$; [111-87-5]	**Original Measurements:** [84]M. E. R. McHale. A. I. Zvaigzne, J. R. Powell, A.-S. M. Kauppila, W. E. Acree, Jr., and S. W. Campbell, Phys. Chem. Liq. **32**, 67 (1996).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 1-octanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.0595	0.0592	0.00522
0.1303	0.1295	0.00629
0.2794	0.2770	0.00853
0.3664	0.3628	0.00978
0.4708	0.4654	0.01154
0.6935	0.6931	0.01506
0.8304	0.8160	0.01736
1.0000	0.9792	0.02077

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.05 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 2-Propanol; C_3H_8O; [67-63-0]
(3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]

Original Measurements:

[85]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; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-propanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00290
0.0774	0.0771	0.00331
0.1578	0.1567	0.00678
0.3137	0.3122	0.00470
0.4145	0.4123	0.00535
0.5187	0.5156	0.00602
0.7251	0.7197	0.00747
0.8573	0.8502	0.00827
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:

(1) Pyrene; $C_{14}H_{10}$; [129-00-0]
(2) 2-Butanol; $C_4H_{12}O$; [78-92-2]
(3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]

Original Measurements:

[85]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; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.0935	0.0931	0.00478
0.1784	0.1775	0.00520
0.3558	0.3537	0.00594
0.4629	0.4599	0.00646
0.5658	0.5619	0.00692
0.7675	0.7614	0.00798
0.8836	0.8759	0.00866
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7] (3) 1-Pentanol; $C_5H_{12}O$; [111-87-5]	[85]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-pentanol + 1-pentanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00640
0.1157	0.1149	0.00679
0.2066	0.2052	0.00701
0.4014	0.3984	0.00755
0.4993	0.4954	0.00789
0.6001	0.5952	0.00816
0.7985	0.7915	0.00872
0.8936	0.8855	0.00909
1.0000	0.9907	0.00931

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-propanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00290
0.0573	0.0571	0.00340
0.1094	0.1090	0.00387
0.2468	0.2455	0.00510
0.3177	0.3159	0.00565
0.4282	0.4254	0.00654
0.6540	0.6484	0.00850
0.8071	0.7989	0.01013
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[87]A. I. Zvaigzne, M. E. R. McHale, J. R. Powell, A.-S. M. Kauppila, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1273 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 2-ethyl-1-hexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.0651	0.0648	0.00485
0.1296	0.1289	0.00531
0.2768	0.2750	0.00651
0.3679	0.3652	0.00723
0.4632	0.4595	0.00804
0.6592	0.6528	0.00968
0.8325	0.8232	0.01118
1.0000	0.9875	0.01250

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[85]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-propanol + cyclohexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00426
0.0781	0.0777	0.00472
0.1516	0.1508	0.00515
0.3047	0.3029	0.00596
0.4046	0.4020	0.00645
0.5200	0.5163	0.00715
0.7425	0.7363	0.00830
0.8714	0.8635	0.00905
1.0000	0.9903	0.00965

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Aldrich Chemical Company.
Component 2 was stored over molecular sieves and distilled shortly before use; Component 3 was stored over molecular sieves and stored at 303.2 K.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[85]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + cyclohexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.0909	0.0903	0.00660
0.1807	0.1794	0.00695
0.3601	0.3574	0.00755
0.4609	0.4572	0.00798
0.5691	0.5644	0.00831
0.7780	0.7710	0.00903
0.8828	0.8746	0.00928
1.0000	0.9903	0.00965

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8%, HPLC grade, Aldrich Chemical Company.
(3) 99%, Aldrich Chemical Company.
Component 2 was stored over molecular sieves and distilled shortly before use; Component 3 was stored over molecular sieves and stored at 303.2 K.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[85]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-methyl-1-propanol + cyclohexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.0856	0.0853	0.00370
0.1616	0.1609	0.00403
0.3421	0.3404	0.00497
0.4516	0.4491	0.00557
0.5570	0.5535	0.00631
0.7691	0.7631	0.00775
0.8821	0.8745	0.00861
1.0000	0.9903	0.00965

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Aldrich Chemical Company.
Component 2 was stored over molecular sieves and distilled shortly before use; Component 3 was stored over molecular sieves and stored at 303.2 K.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

19.4. Pyrene solubility data in binary primary alcohol + tertiary alcohol solvent

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-propanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00426
0.0774	0.0771	0.00435
0.1462	0.1456	0.00442
0.3084	0.3070	0.00469
0.4092	0.4072	0.00491
0.5113	0.5087	0.00507
0.7306	0.7266	0.00552
0.8507	0.8458	0.00579
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.0911	0.0905	0.00618
0.1812	0.1801	0.00616
0.3587	0.3565	0.00620
0.4356	0.4329	0.00618
0.5603	0.5568	0.00620
0.7567	0.7520	0.00617
0.8725	0.8671	0.00619
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-methyl-1-propanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.0970	0.0967	0.00342
0.1808	0.1801	0.00363
0.3659	0.3644	0.00408
0.4755	0.4734	0.00441
0.5696	0.5670	0.00463
0.7668	0.7628	0.00528
0.8703	0.8653	0.00570
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-pentanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00931
0.1101	0.1091	0.00913
0.1955	0.1938	0.00885
0.3939	0.3907	0.00818
0.4866	0.4828	0.00777
0.5989	0.5944	0.00756
0.7969	0.7914	0.00684
0.8883	0.8825	0.00656
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99%, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1276	0.1269	0.00558
0.2134	0.2122	0.00563
0.3988	0.3965	0.00572
0.4997	0.4768	0.00581
0.5912	0.5877	0.00587
0.7903	0.7856	0.00598
0.8931	0.8877	0.00606
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

19.5. Pyrene solubility data in binary secondary alcohol + secondary alcohol solvent

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) 2-Propanol; C_3H_8O; [67-63-0]	[86]A. I. Zvaigzne, B. J. Miller, and W. E. Acree, Jr., J. Chem. Eng. Data **40**, 1267 (1995).
Variables: T/K = 299.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + 2-propanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.1198	0.1193	0.00430
0.2436	0.2426	0.00415
0.4375	0.4358	0.00390
0.5411	0.5391	0.00374
0.6412	0.6389	0.00357
0.8312	0.8285	0.00322
0.9411	0.9382	0.00303
1.0000	0.9971	0.00290

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99+%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[85]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-propanol + cyclohexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00290
0.0701	0.0699	0.00333
0.1412	0.1406	0.00369
0.3172	0.3157	0.00475
0.4155	0.4132	0.00544
0.4844	0.4815	0.00592
0.7325	0.7268	0.00774
0.8429	0.8358	0.00846
1.0000	0.9903	0.00965

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Aldrich Chemical Company.
Component 2 was stored over molecular sieves and distilled shortly before use. Component 3 was stored over molecular sieves and stored at 303.2 K.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[85]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; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + cyclohexanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.0761	0.0757	0.00486
0.1918	0.1908	0.00545
0.3434	0.3413	0.00619
0.4546	0.4515	0.00675
0.5668	0.5626	0.00738
0.7664	0.7599	0.00853
0.8723	0.8644	0.00906
1.0000	0.9903	0.00965

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Aldrich Chemical Company.
Component 2 was stored over molecular sieves and distilled shortly before use.
Component 3 was stored over molecular sieves and stored at 303.2 K.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

19.6. Pyrene solubility data in binary secondary alcohol + tertiary alcohol solvent

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [67-63-0] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-propanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00290
0.0845	0.0842	0.00311
0.1468	0.1463	0.00330
0.3101	0.3089	0.00375
0.4046	0.4030	0.00405
0.5082	0.5060	0.00442
0.7240	0.7203	0.00512
0.8588	0.8540	0.00560
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-pentanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00640
0.0997	0.0991	0.00638
0.2066	0.2053	0.00634
0.3816	0.3792	0.00629
0.5101	0.5069	0.00626
0.6077	0.6039	0.00622
0.8021	0.7971	0.00620
0.8949	0.8893	0.00621
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 4-Methyl-2-pentanol; $C_5H_{12}O$; [108-11-2] (3) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-84-4]	[88]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; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 4-methyl-2-pentanol + 2-methyl-2-butanol mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00621
0.1324	0.1316	0.00623
0.2280	0.2266	0.00626
0.4365	0.4338	0.00628
0.5368	0.5334	0.00629
0.6416	0.6376	0.00626
0.8168	0.8117	0.00626
0.8070	0.8019	0.00621
1.0000	0.9938	0.00617

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, Acros Organics, USA.
(3) 99%, Acros Organics, USA.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.3% (relative error).

20. Solubility of Pyrene in Binary Alcohol + Alkanenitrile Solvent Mixtures

20.1. Critical evaluation of experimental solubility data

Monárrez *et al.*[89] measured the solubility of pyrene binary solvent mixtures containing acetonitrile with 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-pentanol, and 3-methyl-1-butanol at 299.15 K. There has only been a single experimental determination for the solubility of anthracene in each of the binary solvent systems studied. The experimental values were evaluated by curve-fitting the measured solubility data to Eq. (10).

The calculated $S_{23,i}$ parameters for the seven binary alcohol + acetonitrile solvent systems studied are summarized in Table 17, along with the average absolute deviation between the experimental and back-calculated mole fraction solubilities. Examination of the numerical entries in the last column of Table 17 indicates that Eq. (10) does provide a very accurate mathematical representation for how the measured mole fraction solubilities vary with binary solvent composition. Average percent deviations range from 0.8% to 1.1%, indicating that the measured values fall on smooth ln x_1 versus $x_2^{(s)}$ curves. None of the experimental data points was flagged as an outlier.

The experimental pyrene solubility data for binary alcohol + acetonitrile solvent mixtures are tabulated in Sec. 20.2.

TABLE 17. Mathematical representation of pyrene solubilities in binary alcohol (2) + acetonitrile (3) solvent mixtures

Binary solvent system	$S_{23,i}$[a]	% Dev[b]
1-Propanol (2) + acetonitrile (3)	2.698	1.0
	0.860	
	0.217	
2-Propanol (2) + acetonitrile (3)	2.822	1.0
	1.273	
	0.294	
1-Butanol (2) + acetonitrile (3)	3.158	0.8
	0.062	
	0.515	
2-Butanol (2) + acetonitrile (3)	3.539	1.1
	0.908	
	−0.088	
2-Methyl-1-propanol (2) + acetonitrile (3)	3.537	1.0
	0.708	
	−0.136	
2-Pentanol (2) + acetonitrile (3)	3.822	1.0
	−0.011	
	0.476	
3-Methyl-1-butanol (2) + acetonitrile (3)	3.285	1.0
	0.079	
	0.701	

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as $S_{23,0}$, $S_{23,1}$, and $S_{23,2}$.
[b] Dev (%) = $(100/N)\ \Sigma\ |\ [x_1^{\text{exp}} - x_1^{\text{cal}}]/x_1^{\text{exp}}\ |$.

20.2. Pyrene solubility data in binary alcohol + acetonitrile solvent mixtures

Components:	Original Measurements:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Propanol; C_3H_8O; [71-23-8] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-propanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00426
0.1499	0.1488	0.00702
0.2732	0.2708	0.00865
0.4927	0.4878	0.00990
0.5924	0.5866	0.00984
0.6906	0.6842	0.00929
0.8323	0.8257	0.00794
0.9245	0.9181	0.00689
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Propanol; C_3H_8O; [71-23-8] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-propanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00290
0.1619	0.1610	0.00555
0.2662	0.2644	0.00686
0.4903	0.4862	0.00845
0.5636	0.5587	0.00862
0.6684	0.6629	0.00828
0.8408	0.8347	0.00725
0.9241	0.9180	0.00663
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 1-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00622
0.1806	0.1787	0.01034
0.3037	0.3033	0.01217
0.5242	0.5171	0.01363
0.6349	0.6268	0.01280
0.7332	0.7246	0.01179
0.8770	0.8692	0.00886
0.9377	0.9307	0.00748
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00439
0.1711	0.1697	0.00839
0.3252	0.3216	0.01118
0.5339	0.5274	0.01225
0.6346	0.6272	0.01163
0.7300	0.7223	0.01050
0.8762	0.8691	0.00807
0.9412	0.9347	0.00693
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [73-83-1] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-methyl-1-propanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00326
0.1714	0.1703	0.00642
0.3074	0.3047	0.00872
0.5382	0.5324	0.01072
0.6341	0.6274	0.01058
0.7241	0.7169	0.00992
0.8686	0.8616	0.00802
0.9331	0.9324	0.00699
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99.5%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 3-methyl-1-butanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00546
0.1981	0.1961	0.00995
0.3709	0.3664	0.01223
0.5829	0.5753	0.01296
0.6600	0.6517	0.01255
0.7605	0.7519	0.01132
0.8929	0.8853	0.00849
0.9461	0.9392	0.00734
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.
(2) 99+%, anhydrous, Aldrich Chemical Company.
(3) 99.8%, anhydrous, Aldrich Chemical Company.
Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
$x_3^{(s)}$: ±0.0001.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Pyrene; $C_{14}H_{10}$; [129-00-0] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7] (3) Acetonitrile; C_2H_3N; [75-05-8]	[89]C. I. Monárrez, J. H. Woo, P. G. Taylor, A. M. Tran, and W. E. Acree, Jr., J. Chem. Eng. Data **48**, 736 (2003).
Variables:	**Prepared by:**
T/K = 299.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

Solubility of pyrene in 2-pentanol + acetonitrile mixtures[a]

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.00640
0.2222	0.2194	0.01274
0.3733	0.3676	0.01517
0.5690	0.5600	0.01584
0.6652	0.6552	0.01495
0.7626	0.7528	0.01283
0.8900	0.8818	0.00925
0.9494	0.9423	0.00751
1.0000	0.9939	0.00614

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

Auxiliary Information

Method/Apparatus/Procedure:

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

Binary solvent mixtures were prepared by mass. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined by spectrophotometric measurements at 372 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, recrystallized several times from anhydrous methanol.

(2) 99+%, Acros Organics, USA.

(3) 99.8%, anhydrous, Aldrich Chemical Company.

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

Estimated Error:

Temperature: ±0.1 K.

$x_3^{(s)}$: ±0.0001.

x_1: ±1.5% (relative error).

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