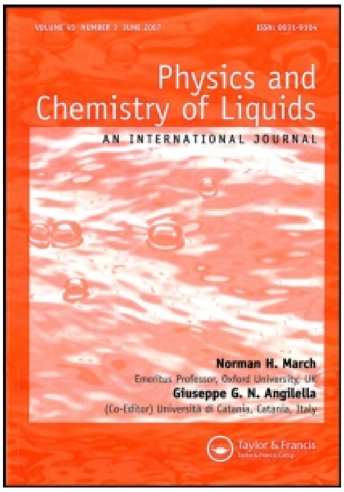

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SOLUBILITY OF ANTHRACENE IN BINARY ALKANE + 2-ETHOXYETHANOL SOLVENT MIXTURES AT 298.2 K

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Experimental solubilities are reported for anthracene dissolved in six binary alkane + 2-ethoxyethanol solvent mixtures at 25°C. The alkane cosolvents studied were hexane, heptane, octane, cyclohexane, methylcyclohexane and 2,2,4-trimethylpentane. Results of these measurements are used to test two mathematical representations based upon the combined Nearly Ideal Binary Solvent (NIBS)/Redlich-Kister and Modified Wilson equations. For the six systems studied, the combined Nearly Ideal Binary Solvent (NIBS)/Redlich-Kister equation provided the better mathematical representation of the experimental data, with an overall average absolute deviation between measured and calculated values being approximately 0.4%. Slightly larger deviations were noted in the case of the Modified Wilson equation.

Keywords: Anthracene solubilities; binary solvent mixtures; alkanes

INTRODUCTION

Solid-liquid equilibrium data of organic nonelectrolyte systems are becoming increasingly important in the petroleum industry, particularly in light of present trends towards heavier feedstocks and known carcinogenicity/matagenicity of many of the larger polycyclic aromatic compounds. Solubility data for a number of polycyclic aromatic

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*Corresponding author. e-mail: acree@unt.edu hydrocarbons (*i.e.*, anthracene and pyrene) and hetero-atom polynuclear aromatics (*i.e.*, carbazole, dibenzothiophene and xanthene) have been published in the recent chemical literature (for listing of references see Acree [1 – 3]). Despite efforts by experimentalists and scientific organizations, both in terms of new experimental measurements and critically-evaluated data compilations, there still exist numerous systems for which solubility data are not readily available.

To address this problem, researchers have turned to predictive methods as a means to generate desired quantities. Numerous equations have been suggested for predicting solute solubilities in binary solvent mixtures. For the most part, the predictive methods do provide fairly reasonable estimates for non-complexing systems. There still remains, however, the need to develop better predictive expressions and mixing models to describe the more nonideal complexing systems believed to contain hydrogen bonding solvent components. Continued development of solution models for describing the thermodynamic properties of a solute in binary solvent systems requires that a large data base be available for assessing the applications and limitations of derived expressions. Currently, only a limited data base exists for crystalline nonelectrolyte solubility in binary solvent mixtures. For this reason, anthracene solubilities were determined in six binary alkane + 2-ethoxyethanol solvent mixtures. Results of these measurements are used to further test the descriptive abilities of two previously derived expressions.

EXPERIMENTAL METHODS

Anthracene (Acros, 99.9 + %) was recrystallized three times from 2-propanone. 2-Ethoxyethanol (Aldrich, 99%), hexane (Aldrich, 99 + %), heptane (Aldrich, HPLC), octane (Aldrich, 99 + %, anhydrous), cyclohexane (Aldrich, HPLC), methylcyclohexane (Aldrich, 99 + %, anhydrous) and 2,2,4-trimethylpentane (Aldrich, HPLC) were stored over molecular sieves and distilled shortly before use. Gas chromatographic analysis showed solvent purities to be 99.7 mole percent or better. Binary solvent mixtures were prepared by mass so that compositions could be calculated to 0.0001 mole fraction.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate in a constant temperature water bath at

(25.0 ± 0.1)°C with periodic agitation for at last three days (often longer). Attainment of equilibrium was verified both by repetitive measurements after a minimum of three additional days and by approaching equilibrium from supersaturation by pre-equilibrating the solutions at a higher temperature. Aliquots of saturated anthracene solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with methanol for spectrophotomeric analysis of 356 nm on a Bausch and Lomb Spectronic 2000. Concentrations of the dilute solutions were determined from a Beer–Lambert law absorbance *versus* concentration working curve derived from measured absorbances of standard solutions of known molar concentration. Apparent molar absorptivities of the nine standard solutions varied systematically with molar concentration, and ranged from approximately $\varepsilon/(\text{Liter mol}^{-1}\text{cm}^{-1}) = 7450$ to $\varepsilon/(\text{Liter mol}^{-1}\text{cm}^{-1}) = 7150$ for anthracene concentrations ranging from $C/(\text{mol L}^{-1}) = 6.75 \times 10^{-5}$ to $C/(\text{mol L}^{-1}) = 2.25 \times 10^{-4}$. Identical molar absorptivities were obtained for select anthracene standard solutions that contained up to 5 volume percent of the neat alkane and 2-ethoxyethanol cosolvents. Experimental anthracene solubilities in the six binary alkane + 2-ethoxyethanol solvent mixtures are listed in Table I. Numerical values represent the average of between four and eight independent determinations, with the measured values being reproducible to within ± 1.5%.

RESULTS AND DISCUSSION

Acree and Zvaigzne [4] suggested possible mathematical representations for isothermal solubility data based upon either a Combined NIBS/Redlich-Kister model

$$\ln x_A^{\text{sat}} = x_B^{\circ} \ln(x_A^{\text{sat}})_B + x_C^{\circ} \ln(x_A^{\text{sat}})_C + x_B^{\circ} x_C^{\circ} \sum_{i=0}^{N} S_i (x_B^{\circ} - x_C^{\circ})^i \qquad (1)$$

or Modified Wilson equation

$$\begin{aligned} \ln[a_A(s)/x_A^{\text{sat}}] = 1 &- x_B^{\circ}\{1 - \ln[a_A(s)/(x_A^{\text{sat}})_B]\}/(x_B^{\circ} + x_C^{\circ}\Lambda_{BC}^{\text{adj}}) \\ &- x_C^{\circ}\{1 - \ln[a_A(s)/(x_A^{\text{sat}})_C]\}/(x_B^{\circ}\Lambda_{CB}^{\text{adj}} + x_C^{\circ}) \qquad (2) \end{aligned}$$

TABLE I Experimental mole fraction solubilities of anthracene (x_A^{sat}) in binary alkane (B) + 2-ethoxyethanol (C) solvent mixtures at 25.0°C

x_C^o	x_A^{sat}
Hexane (B) + 2-ethoxyethanol (C)	
0.0000	0.001274
0.1278	0.001740
0.2647	0.002157
0.4837	0.002698
0.5851	0.002947
0.6786	0.003106
0.8386	0.003158
0.9340	0.003074
1.0000	0.002921
Heptane (B) + 2-ethoxyethanol (C)	
0.0000	0.001571
0.1583	0.002085
0.2787	0.002402
0.5044	0.002920
0.6029	0.003109
0.6998	0.003229
0.8573	0.003276
0.9265	0.003152
1.0000	0.002921
Octane (B) + 2-ethoxyethanol (C)	
0.0000	0.001838
0.1779	0.002397
0.2987	0.002703
0.5246	0.003146
0.6224	0.003278
0.7186	0.003376
0.8679	0.003293
0.9315	0.003173
1.0000	0.002921
Cyclohexane (B) + 2-ethoxyethanol (C)	
0.0000	0.001553
0.1151	0.002076
0.2195	0.002461
0.4346	0.003051
0.5300	0.003238
0.6247	0.003321
0.8151	0.003287
0.9033	0.003142
1.0000	0.002921
Methylcyclohexane (B) + 2-ethoxyethanol (C)	
0.0000	0.001649
0.1224	0.002196
0.2531	0.002604
0.4700	0.003059
0.5775	0.003224
0.6745	0.003313

TABLE I (Continued)

x_C°	x_A^{sat}
0.8452	0.003266
0.9181	0.003134
1.0000	0.002921
2,2,4-Trimethylpentane (B) + 2-ethoxyethanol (C)	
0.0000	0.001074
0.1778	0.001528
0.3156	0.001885
0.5317	0.002420
0.6207	0.002609
0.7288	0.002859
0.8670	0.003020
0.9376	0.003013
1.0000	0.002921

TABLE II Mathematical representation of anthracene solubilities in several binary alkane (B) + 2-ethoxyethanol (C) solvent mixtures

Binary solvent system	*Eq.* (1)		*Eq.* (2)	
component (*B*) + *component* (*C*)	S_i [a]	% *Dev.* [b]	Λ_{ij}^{adj}, [c]	% *Dev.* [b]
Hexane + 2-ethoxyethanol	1.434	0.6	2.960	1.0
	0.126		10.130	
	0.526			
Heptane + 2-ethoxyethanol	1.220	0.2	2.900	1.5
	−0.168		12.970	
	0.594			
Octane + 2-ethoxyethanol	1.158	0.3	3.230	1.6
	−0.205		15.390	
	0.571			
Cyclohexane + 2-ethoxyethanol	1.606	0.5	4.332	2.8
	0.354		12.990	
	0.374			
Methylcyclohexane + 2-ethoxyethanol	1.410	0.6	5.739	2.3
	0.289		9.450	
	0.613			
2,2,4-Trimethylpentane + 2-ethoxyethanol	1.101	0.3	1.990	0.6
	−0.134		6.970	
	0.475			

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as S_0, S_1 and S_2;
[b] Deviation(%) = $(100/N)\Sigma|[(x_A^{\text{sat}})^{\text{calc}} - (x_A^{\text{sat}})^{\text{exp}}]/(x_A^{\text{sat}})^{\text{exp}}|$;
[c] Adjustable parameters for the Modified Wilson equation are ordered as $\Lambda_{BC}^{\text{adj}}$ and $\Lambda_{CB}^{\text{adj}}$.

where the various S_i and $\Lambda_{ij}^{\text{adj}}$ "curve-fit" parameters can be evaluated *via* least squares analysis. In Eqs. (1) and (2) x_B° and x_C° refer to the initial mole fraction composition of the binary solvent calculated as if solute (A) were not present, $a_A(s)$ is the activity of the solid solute, N is the number of curve-fit parameters used, and $(x_A^{\mathrm{sat}})_i$ is the saturated mole fraction solubility of the solute in pure solvent i. The numerical value of $a_A(s)$ used in the Modified Wilson computations was $a_A(s) = 0.00984$ [5].

The ability of Eqs. (1) and (2) to mathematically represent the experimental solubility of anthracene in the six binary alkane + 2-ethoxyethanol mixtures is summarized in Table II in the form of "curve-fit" parameters and percent deviations in back-calculated solubilities. Each percent deviation is based upon the measured anthracene solubility data at the seven different binary solvent compositions. Careful examination of Table II reveals that both equations provide a fairly accurate mathematical representation for how the solubility of anthracene varies with solvent composition. For the six anthracene systems studied, Eq. (1) was found to provide the better description of the experimental data, with the overall average absolute deviation between the observed and calculated values being approximately ±0.4%, which is less than the experimental uncertainty. Slightly larger deviations were noted in the case of Eq. (2).

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