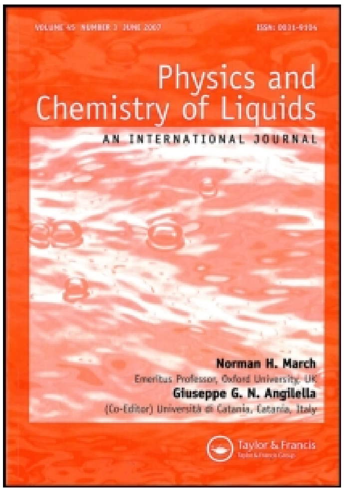

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SOLUBILITY OF *TRANS*-STILBENE IN BINARY ALKANE + 1-BUTANOL SOLVENT MIXTURES AT 298.2 K

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Experimental solubilities are reported for *trans*-stilbene dissolved in six binary alkane + 1-butanol 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 NIBS/Redlich-Kister equation was found to provide the better mathematical representation of the experimental data, with overall average absolute deviations between measured and calculated values being approximately ±0.6%. Slightly larger deviations were noted in the case of the Modified Wilson equation.

Keywords and Phrases: Trans-stilbene 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/mutagenicity 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, *trans*-stilbene solubilities were determined in six binary alkane + 1-butanol solvent mixtures. Results of these measurements are used to further test the descriptive abilities of two previously derived expressions.

EXPERIMENTAL METHODS

Trans-stilbene (Aldrich, 96%) was recrystallized three times from methanol. 1-Butanol (Aldrich, 99.8 + %, anhydrous), 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 least 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 *trans*-stilbene solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with methanol for spectrophotometric analysis at 294 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 ranging from 1.38×10^{-5} Molar to 4.62×10^{-5} Molar. The calculated molar absorptivity of $\epsilon \approx 28{,}850$ Liter $\mathrm{mol}^{-1}\,\mathrm{cm}^{-1}$ was constant over the concentration range. Identical molar absorptivities were obtained for select *trans*-stilbene standard solutions that contained up to 5 volume percent of the neat alkane and 1-butanol cosolvents. Experimental *trans*-stilbene solubilities in the six binary alkane + 1-butanol 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%.

TABLE I Experimental mole fraction solubilities of *trans*-stilbene (x_A^{sat}) in binary alkane (B) + 1-Butanol (C) solvent mixtures at 25.0°C

x_C^o	x_A^{sat}
Hexane (B) + 1-Butanol (C)	
0.0000	0.00960
0.1578	0.01035
0.2704	0.01021
0.4883	0.00906
0.5906	0.00831
0.6973	0.00758
0.8486	0.00647
0.9171	0.00594
1.0000	0.00533

TABLE I (Continued)

x_C^o	x_A^{sat}
Heptane (*B*) + 1-Butanol (*C*)	
0.0000	0.01085
0.1601	0.01149
0.2950	0.01083
0.5167	0.00961
0.6169	0.00874
0.7028	0.00833
0.8672	0.00674
0.9268	0.00613
1.0000	0.00533
Octane (*B*) + 1-Butanol (*C*)	
0.0000	0.01241
0.1863	0.01233
0.3174	0.01156
0.5342	0.01008
0.6436	0.00910
0.7299	0.00835
0.8739	0.00707
0.9428	0.00619
1.0000	0.00533
Cyclohexane (*B*) + 1-Butanol (*C*)	
0.0000	0.01374
0.1337	0.01414
0.2331	0.01341
0.4347	0.01161
0.5440	0.01029
0.6439	0.00934
0.8219	0.00740
0.9081	0.00640
1.0000	0.00533
Methylcyclohexane (*B*) + 1-Butanol (*C*)	
0.0000	0.01413
0.1450	0.01405
0.2757	0.01327
0.4858	0.01135
0.5942	0.01058
0.6826	0.00952
0.8341	0.00756
0.9181	0.00651
1.0000	0.00533
2,2,4-Trimethylpentane (*B*) + 1-Butanol (*C*)	
0.0000	0.00803
0.1808	0.00852
0.3281	0.00857
0.5413	0.00815
0.6437	0.00771
0.7300	0.00739
0.8684	0.00645
0.9388	0.00595
1.0000	0.00533

RESULTS AND DISCUSSION

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

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

or Modified Wilson equation

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

where the various S_i and $\Lambda_{ij}^{\mathrm{adj}}$ "curve-fit" parameters can be evaluated *via* least squares analysis. In Eqs. (1) and (2) x_B^o and x_C^o 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 $a_A(s) = 0.06227$ [5].

The ability of Eqs. (1) and (2) to mathematically represent the experimental solubility of *trans*-stilbene in the six binary alkane + 1-butanol 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 *trans*-stilbene solubility data at the seven different binary solvent compositions. Careful examination of Table II reveals that both equations provided a fairly accurate mathematical representation for how the solubility of *trans*-stilbene varies with solvent composition. For the six *trans*-stilbene systems studied, Eq. (1) was found to provide the better mathematical representation of the experimental data. Deviations between the experimental mole fraction solubilities and back-calculated values based upon Eq. (1) differed by an overall average absolute deviation of about ± 0.6%, which is less than the experimental uncertainty. Slightly larger deviations were noted in the case of Eq. (2).

TABLE II Mathematical representation of *trans*-stilbene solubilities in several binary alkane (B) + 1-Butanol (C) solvent mixtures

Binary Solvent System *Component* (B) + *Component* (C)	*Eq.* (1) S_i^{a}	 % *Dev.*[b]	*Eq.* (2) $\Lambda_{ij}^{adj,c}$	 % *Dev.*[b]
Hexane + 1-Butanol	0.910	0.1	2.594	0.4
	0.342		1.115	
	0.254			
Heptane + 1-Butanol	0.968	0.8	1.463	1.4
	0.033		1.724	
	0.518			
Octane + 1-Butanol	0.878	0.8	1.231	1.6
	−0.311		1.840	
	0.874			
Cyclohexane + 1-Butanol	0.945	0.5	2.710	1.2
	0.127		1.434	
	0.496			
Methylcyclohexane + 1-Butanol	1.078	0.7	1.492	0.9
	−0.262		1.956	
	0.386			
2,2,4-Trimethylpentane + 1-Butanol	0.909	0.5	1.173	0.8
	−0.215		1.753	
	0.399			

[a] Combined NIBS/Redlich-Kister curve-fit parameters are ordered as S_0, S_1 and S_2.

[b] Deviation (%) = $(100/N)\sum|[(x_A^{sat}) - (x_A^{sat})^{exp}]/(x_A^{sat})^{exp}|$.

[c] Adjustable parameters for the Modified Wilson equation are ordered as Λ_{BC}^{adj} and Λ_{CB}^{adj}.

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