

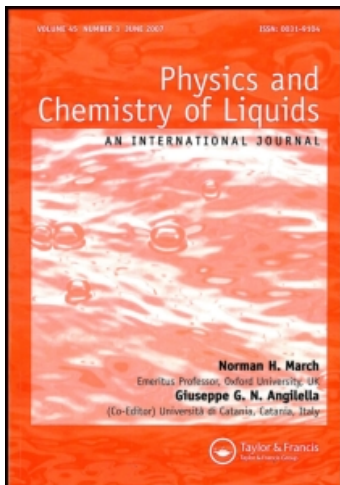
This article was downloaded by:

On: 28 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Physics and Chemistry of Liquids

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713646857>

Solubility of Anthracene in Binary Alkane 2-Methyl-2-Propanol Solvent Mixtures at 298.2 K

Karina M. De Fina^a; Tiffany T. Van^a; Andres Ibarra^a; Eboney Hamilton^a; Josh Martinez^a; Alison Valdez^a; William E. Acree Jr.^a

^a Department of Chemistry, University of North Texas, Denton, Texas, USA

To cite this Article De Fina, Karina M. , Van, Tiffany T. , Ibarra, Andres , Hamilton, Eboney , Martinez, Josh , Valdez, Alison and Acree Jr., William E.(2001) 'Solubility of Anthracene in Binary Alkane 2-Methyl-2-Propanol Solvent Mixtures at 298.2 K', *Physics and Chemistry of Liquids*, 39: 2, 249 – 254

To link to this Article: DOI: 10.1080/00319100108030343

URL: <http://dx.doi.org/10.1080/00319100108030343>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

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

KARINA M. DE FINA, TIFFANY T. VAN, ANDRES IBARRA,
EBONEY HAMILTON, JOSH MARTINEZ, ALISON VALDEZ
and WILLIAM E. ACREE JR.*

*Department of Chemistry, University of North Texas, Denton,
Texas 76203-5070, USA*

(Received 17 March 2000)

Experimental solubilities are reported for anthracene dissolved in four binary alkane + 2-methyl-2-propanol solvent mixtures at 25°C. The alkane cosolvents studied were *n*-heptane, 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 four 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 $\pm 0.5\%$. Slightly larger deviations were noted in the case of the Modified Wilson equation.

Keywords and Phrases: Anthracene solubilities; Binary solvent mixtures; Alkane cosolvents

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

*Corresponding author. e-mail: acree@unt.edu

hydrocarbons (*i.e.*, anthracene and pyrene) and hetero-atom polynuclear aromatics (*i.e.*, carbazole, dibenzothiophene and xanthenes) 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 noncomplexing 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 four binary alkane + 2-methyl-2-propanol solvent mixtures. Results of these measurements are used to further test the descriptive abilities of two previously derived expressions.

EXPERIMENTAL METHODS

Anthracene (Aldrich, 99.9+%) was used as received. *n*-Heptane (Aldrich, HPLC), cyclohexane (Aldrich, HPLC), methylcyclohexane (Aldrich, 99+%, anhydrous), 2,2,4-trimethylpentane (Aldrich, HPLC) and 2-methyl-2-propanol (Arco Chemical Company, 99+%) 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

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

x_C^0	x_A^{sat}
<i>n</i>-Heptane (B) + 2-Methyl-2-propanol (C)	
0.0000	0.001571
0.1354	0.001536
0.2898	0.001382
0.5125	0.001137
0.5993	0.001025
0.7060	0.000892
0.8485	0.000677
0.9172	0.000570
1.0000	0.000430
Cyclohexane (B) + 2-Methyl-2-propanol (C)	
0.0000	0.001553
0.1213	0.001553
0.2219	0.001446
0.4242	0.001187
0.5264	0.001074
0.6314	0.000933
0.8199	0.000677
0.9072	0.000555
1.0000	0.000430
Methylcyclohexane (B) + 2-Methyl-2-propanol (C)	
0.0000	0.001649
0.1382	0.001632
0.2612	0.001506
0.4844	0.001200
0.5682	0.001086
0.6681	0.000940
0.8386	0.000669
0.9143	0.000553
1.0000	0.000430
2,2,4-Trimethylpentane (B) + 2-Methyl-2-propanol (C)	
0.0000	0.001074
0.1655	0.001049
0.3092	0.000972
0.5406	0.000847
0.6368	0.000781
0.6887	0.000747
0.8761	0.000569
0.9321	0.000507
1.0000	0.000430

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 spectrophotometric analysis at 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 concentrations. The calculated molar absorptivities of the nine standard solutions varied systematically with molar concentration and ranged from approximately $\epsilon \approx 7450 \text{ Liter mol}^{-1} \text{ cm}^{-1}$ to $\epsilon \approx 7150 \text{ Liter mol}^{-1} \text{ cm}^{-1}$ for anthracene concentrations ranging from $C = 6.75 \times 10^{-5} \text{ Molar}$ to $C = 2.25 \times 10^{-4} \text{ Molar}$. Experimental anthracene solubilities in the four binary alkane + 2-methyl-2-propanol 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 $\pm 1.5\%$.

RESULTS AND DISCUSSION

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

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

or Modified Wilson equation

$$\ln \left[a_A(s) / x_A^{\text{sat}} \right] = 1 - x_B^0 \left\{ 1 - \ln \left[a_A(s) / (x_A^{\text{sat}})_B \right] \right\} / \left(x_B^0 + x_C^0 \Lambda_{BC}^{\text{adj}} \right) - x_C^0 \left\{ 1 - \ln \left[a_A(s) / (x_A^{\text{sat}})_C \right] \right\} / \left(x_B^0 \Lambda_{CB}^{\text{adj}} + x_C^0 \right) \quad (2)$$

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^0 and x_C^0 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

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

Binary solvent system	Eq. (1)		Eq. (2)	
	S_i^a	%Dev. ^b	$\Lambda_{ij}^{adj,c}$	%Dev. ^b
<i>n</i> -Heptane + 2-Methyl-2-propanol	1.326 -0.547 0.702	0.3	0.535 2.536	1.0
Cyclohexane + 2-Methyl-2-propanol	1.189 -0.118 0.544	0.7	0.941 1.840	1.4
Methylcyclohexane + 2-Methyl-2-propanol	1.373 -0.165 0.369	0.5	1.463 1.724	1.0
2,2,4-Trimethylpentane + 2-Methyl-2-propanol	1.003 -0.411 0.379	0.3	0.593 2.246	0.5

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

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

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

the number of curve-fit parameters used, and $(x_A^{\text{sat}})_i$ 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 four alkane+2-methyl-2-propanol 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 provided a fairly accurate mathematical representation for how the solubility of anthracene varies with solvent composition. For the four anthracene 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 $\pm 0.5\%$, which is less than the experimental uncertainty. Slightly larger deviations were noted in the case of Eq. (2).

Acknowledgements

Andres Ibarra, Eboney Hamilton, Josh Martinez and Alison Valdez thank the U.S. Department of Education for support provided to them under the Upward Bound Math and Science Program.

References

- [1] Acree, W. E. Jr. (1994). Polycyclic Aromatic Hydrocarbons in Pure and Binary Solvents. Vol. 54, In: *IUPAC Solubility Data Series*, Oxford University Press: Oxford, United Kingdom.
- [2] Acree, W. E. Jr. (1995). Polycyclic Aromatic Hydrocarbons: Binary Nonaqueous Systems: Part 1 (Solutes A-E). Vol. 58, In: *IUPAC Solubility Data Series*, Oxford University Press: Oxford, United Kingdom.
- [3] Acree, W. E. Jr. (1995). Polycyclic Aromatic Hydrocarbons: Binary Nonaqueous Systems: Part 2 (Solutes F-Z). Vol. 59, In: *IUPAC Solubility Data Series*, Oxford University Press: Oxford, United Kingdom.
- [4] Acree, W. E. Jr. and Zvaigzne, A. I. (1991). *Thermochim. Acta*, **178**, 151.
- [5] Powell, J. R., Coym, K. S. and Acree, W. E. Jr. (1997). *J. Chem. Eng. Data*, **42**, 395.