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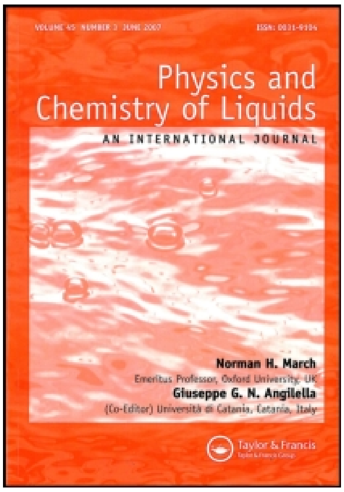

**Physics and Chemistry of Liquids**
Publication details, including instructions for authors and subscription information:
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# Solubility of Anthracene in Binary p-xylene Alkane and Benzene Alkane Solvent Mixtures

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**To cite this Article** Acree Jr., William E. and Tucker, Sheryl A.(1989) 'Solubility of Anthracene in Binary p-xylene Alkane and Benzene Alkane Solvent Mixtures', Physics and Chemistry of Liquids, 20: 1, 31 — 38

**To link to this Article: DOI:** 10.1080/00319108908031697

**URL:** http://dx.doi.org/10.1080/00319108908031697

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*Phys. Chem. Liq.*, 1989, Vol. 20, pp. 31-38
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# SOLUBILITY OF ANTHRACENE IN BINARY *p*-XYLENE + ALKANE AND BENZENE + ALKANE SOLVENT MIXTURES

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*(Received 15 October 1988)*

Experimental solubilities are reported for anthracene in binary solvent mixtures containing *p*-xylene with *n*-hexane, *n*-heptane, *n*-octane, methylcyclohexane, cyclohexane and isooctane, and benzene with *n*-octane and methylcyclohexane at 25°C. Results of these measurements are used to test five predictive expressions derived from the Nearly Ideal Binary Solvent (NIBS) model. The most successful equation in terms of goodness of fit involved a surface fraction average of the excess partial molar Gibbs free energy of the solute relative to Raoult's law and predicted the experimental anthracene solubilities in the 8 systems studied to within an average absolute deviation of 3.8%.

KEY WORDS: Anthracene solubilities-binary solvents, binary solvents, solid-liquid equilibria.

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## INTRODUCTION

Solid-liquid equilibrium data of organic systems are becoming increasingly important in the petroleum industry, particularly in light of present trends towards heavier feed stock and coal-derived fuels. Solubility data for a number of polycyclic aromatic hydrocarbons[1-5] (i.e., anthracene and pyrene) and heterocyclic polynuclear aromatics[6-8] (i.e., carbazole, dibenzothiophene and xanthene) have been published in recent chemical literature. Despite efforts by experimentalists and scientific organizations, both in terms of new experimental measurements and critically-evaluated data compilations, there still exists numerous systems for which actual solubility data are not readily available.

To address this problem, researchers have turned to group contribution methods and semi-empirical expressions to predict desired quantities. Group contribution methods have proved fairly successful in estimating solid solubility in pure and binary solvent mixtures from structural information.[9-16] Practical application, though, is limited to systems for which all group interaction parameters are known. Generally,

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interaction parameters are evaluated from solid-liquid and liquid-vapor equilibria data, and it is important that the data base contain as many of the different functional groups as possible. The data base should contain sufficient experimental values near infinite dilution in the event that one wishes to determine separate interaction parameters for finite concentration and for infinite dilution activity coefficient predictions. The UNIFAC model[17] now has two sets of group interaction parameters, with the recent publication of the infinite dilution values by Bastos *et al.*[18]

Predictive expressions for solid-liquid equilibria have also been derived from simple thermodynamic mixing models. The Nearly Ideal Binary Solvent (NIBS) model developed previously[19–21] provides a relatively simple method for estimating the excess partial molar properties of a solute, $\bar{Z}_3^{\mathrm{ex}}$, at infinite dilution in a binary solvent (components 1 and 2):

$$\bar{Z}_3^{\mathrm{ex}} = f_1^0(\bar{Z}_3^{\mathrm{ex}})_1 + f_2^0(\bar{Z}_3^{\mathrm{ex}})_2 - \Gamma_3(X_1^0\Gamma_1 + X_2^0\Gamma_2)^{-1}\bar{Z}_{12}^{\mathrm{ex}} \tag{1}$$
$$f_1^0 = 1 - f_2^0 = X_1^0\Gamma_1/(X_1^0\Gamma_1 + X_2^0\Gamma_2)$$

in terms of a weighted mole fraction average of the properties of the solute in the two pure solvents, $(\bar{Z}_3^{\mathrm{ex}})_1$ and $(\bar{Z}_3^{\mathrm{ex}})_2$, and a contribution due to the unmixing of the solvent pair by the presence of the solute. Equation 1 (with $\bar{Z}^{\mathrm{ex}} = \bar{G}^{\mathrm{ex}}$) gives accurate predictions for naphthalene, iodine, *p*-dibromobenzene, benzil, *p*-benzoquinone, benzoic acid and phenylacetic acid solubilities in systems of nonspecific interactions when molar volumes are used as weighting factors ($\Gamma_i$).[21] Approximation of weighting factors with molecular surface areas enables Eq. (1) to provide accurate predictions for anthracene[1] and pyrene[3] solubilities in binary solvent mixtures containing benzene. The NIBS model has also served as the point-of-departure for the development of thermodynamic expressions for describing ternary associated solutions in which the solute complexes with a single or with both solvent components.[6,7,22–24]

Continued development of solution models for predicting 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 predictive expressions. Currently, only a limited data base exists for crystalline nonelectrolyte solubility in binary solvent systems. For this reason, anthracene solubilities were determined in mixtures containing *p*-xylene with *n*-hexane, *n*-heptane, *n*-octane, cyclohexane, methylcyclohexane and isooctane, which cover up to a sevenfold range in mole fraction solubilities. Anthracene solubilities were also measured in binary benzene + methylcyclohexane and benzene + *n*-octane mixtures to supplement the experimental data previously reported.[1] Results of these measurements are compared to predictions of the NIBS model.

## MATERIALS AND METHODS

Anthracene (Aldrich Gold Label) was used as received. Cyclohexane (Aldrich HPLC), *n*-heptane (Aldrich HPLC), *n*-hexane (Aldrich 99%), *n*-octane (Aldrich Gold Label), isooctane (Aldrich HPLC), methylcyclohexane (Aldrich Gold Label), benzene (Aldrich HPLC) and *p*-xylene (Aldrich HPLC) were stored over molecular sieves to

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remove trace water. Gas chromatographic analysis showed solvent purities to be 99.8% or better. Binary solvent mixtures were prepared by weight 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 bath at 25.0 ± 0.1°C for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days and in some instances by approaching equilibrium from supersaturation by preequilibrating the solutions at a higher temperature. Aliquots of saturated solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with methanol. Concentrations were determined spectrophotometrically at 356 nm on a Bausch and Lomb Spectronic 2000. Experimental solubilities are listed in Table 1. Numerical values represent the average of 4–8 independent determinations, with measurements being reproducible to ±1%. Solubilities in the pure alkane solvents are in excellent agreement with earlier values of Acree and Rytting.[1]

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## RESULTS AND DISCUSSION

The general NIBS expressions for predicting solubilities in systems of nonspecific interactions depend on different models of solution ideality and weighting factor approximations:

$$RT\ln(a_3^{\text{solid}}/X_3^{\text{sat}}) = (1 - X_3^{\text{sat}})^2[X_1^0(\bar{G}_3^{\text{ex}})_1 + X_2^0(\bar{G}_3^{\text{ex}})_2 - \bar{G}_{12}^{\text{ex}}] \qquad \text{(XX)}$$

$$\begin{aligned} RT\ln(a_3^{\text{solid}}/X_3^{\text{sat}}) = {} & (1 - \phi_3^{\text{sat}})^2[\phi_1^0(\bar{G}_3^{\text{ex}})_1 + \phi_2^0(\bar{G}_3^{\text{ex}})_2 \\ & - \bar{V}_3(X_1^0\bar{V}_1 + X_2^0\bar{V}_2)^{-1}\bar{G}_{12}^{\text{ex}}] \end{aligned} \qquad \text{(XV)}$$

$$\begin{aligned} RT\ln(a_3^{\text{solid}}/X_3^{\text{sat}}) = {} & (1 - \theta_3^{\text{sat}})^2[\theta_1^0(\bar{G}_3^{\text{ex}})_1 + \theta_2^0(\bar{G}_3^{\text{ex}})_2 \\ & - \bar{A}_3(X_1^0\bar{A}_1 + X_2^0\bar{A}_2)^{-1}\bar{G}_{12}^{\text{ex}}] \end{aligned} \qquad \text{(XA)}$$

$$\begin{aligned} & RT\left[\ln(a_3^{\text{solid}}/\phi_3^{\text{sat}}) - (1 - \phi_3^{\text{sat}})\left(1 - \frac{\bar{V}_3}{X_1^0\bar{V}_1 + X_2^0\bar{V}_2}\right)\right] \\ & \quad = (1 - \phi_3^{\text{sat}})^2[\phi_1^0(\bar{G}_3^{\text{fh}})_1 + \phi_2^0(\bar{G}_3^{\text{fh}})_2 - \bar{V}_3(X_1^0\bar{V}_1 + X_2^0\bar{V}_2)^{-1}\bar{G}_{12}^{\text{fh}}] \end{aligned} \qquad \text{(VV)}$$

$$\begin{aligned} & RT\left[\ln(a_3^{\text{solid}}/\phi_3^{\text{sat}}) - (1 - \phi_3^{\text{sat}})\left(1 - \frac{\bar{V}_3}{X_1^0\bar{V}_1 + X_2^0\bar{V}_2}\right)\right] \\ & \quad = (1 - \theta_3^{\text{sat}})^2[\theta_1^0(\bar{G}_3^{\text{fh}})_1 + \theta_2^0(\bar{G}_3^{\text{fh}})_2 - \bar{A}_3(X_1^0\bar{A}_1 + X_2^0\bar{A}_2)^{-1}\bar{G}_{12}^{\text{fh}}] \end{aligned} \qquad \text{(VA)}$$

Equations (XX), (XV) and (XA) are based on Raoult's law while Eqs. (VV) and (VA) are based on the Flory–Huggins model. In the above expressions $\bar{V}_i$ is the molar volume of a pure liquid, $\bar{A}_i$ is the molecular surface area, $X_i$ denotes mole fraction, $\phi_i$ is volume fraction, $\theta_i$ is surface fraction, $\bar{G}_{12}^{\text{ex}}$ refers to the molar excess Gibbs free energy of the binary solvent relative to Raoult's law, and

$$\bar{G}_{12}^{\text{fh}} = \bar{G}_{12}^{\text{ex}} + RT[\ln(X_1^0\bar{V}_1 + X_2^0\bar{V}_2) - X_1^0\ln\bar{V}_1 - X_2^0\ln\bar{V}_2]$$

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**Table 1** Mole fraction solubility of anthracene in several binary *p*-xylene + alkane and benzene + alkane solvent mixtures at 25°C.

| *Solvent* (1) + *Solvent* (2) | $X_1^0$ | $X_3^{sat}$ |
|---|---|---|
| *n*-Hexane + *p*-Xylene | 0.0000 | 0.00733 |
| | 0.1945 | 0.00602 |
| | 0.3807 | 0.00459 |
| | 0.4823 | 0.00388 |
| | 0.5882 | 0.00327 |
| | 0.7833 | 0.00222 |
| | 1.0000 | 0.00127 |
| *n*-Heptane + *p*-Xylene | 0.0000 | 0.00733 |
| | 0.1747 | 0.00593 |
| | 0.3547 | 0.00463 |
| | 0.4490 | 0.00403 |
| | 0.5571 | 0.00341 |
| | 0.7648 | 0.00240 |
| | 1.0000 | 0.00157 |
| *n*-Octane + *p*-Xylene | 0.0000 | 0.00733 |
| | 0.1631 | 0.00621 |
| | 0.3491 | 0.00494 |
| | 0.4395 | 0.00431 |
| | 0.5346 | 0.00376 |
| | 0.7454 | 0.00274 |
| | 1.0000 | 0.00184 |
| Cyclohexane + *p*-Xylene | 0.0000 | 0.00733 |
| | 0.2232 | 0.00610 |
| | 0.4303 | 0.00485 |
| | 0.5304 | 0.00417 |
| | 0.6322 | 0.00357 |
| | 0.8137 | 0.00251 |
| | 1.0000 | 0.00155 |
| Methylcyclohexane + *p*-Xylene | 0.0000 | 0.00733 |
| | 0.2045 | 0.00592 |
| | 0.3822 | 0.00482 |
| | 0.4879 | 0.00418 |
| | 0.5939 | 0.00360 |
| | 0.7977 | 0.00252 |
| | 1.0000 | 0.00165 |
| Isooctane + *p*-Xylene | 0.0000 | 0.00733 |
| | 0.1626 | 0.00577 |
| | 0.3333 | 0.00430 |
| | 0.4311 | 0.00357 |
| | 0.5334 | 0.00293 |
| | 0.7484 | 0.00186 |
| | 1.0000 | 0.00107 |
| *n*-Octane + Benzene | 0.0000 | 0.00742 |
| | 0.1227 | 0.00616 |
| | 0.2606 | 0.00508 |
| | 0.3524 | 0.00444 |
| | 0.4575 | 0.00377 |
| | 0.6838 | 0.00280 |
| | 0.8156 | 0.00239 |
| | 1.0000 | 0.00184 |
| Methylcyclohexane + Benzene | 0.0000 | 0.00742 |
| | 0.1519 | 0.00625 |
| | 0.3209 | 0.00504 |
| | 0.4098 | 0.00440 |
| | 0.5257 | 0.00370 |
| | 0.7353 | 0.00267 |
| | 1.0000 | 0.00165 |

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The superscript (0) indicates that the solvent composition is calculated as if the solute were not present. The activity of the solid solute ($a_3^{solid}$), relative to the supercooled liquid, can be calculated from

$$\ln a_3^{solid} = -\frac{\Delta\bar{H}_3^{fus}(T_m - T)}{RT\,T_m} + \frac{\Delta\bar{C}_p(T_m - T)}{RT} - (\Delta\bar{C}_p/R)\ln(T_m/T)$$

the molar heat of fusion ($\Delta\bar{H}_3^{fus}$) at the normal melting point temperature ($T_m$) and the difference between the molar heat capacities of the liquid and solid.

The predictive ability of the five NIBS expressions is summarized in Table 2. For three of the binary systems studied, methylcyclohexane + benzene,[25] *n*-octane + benzene[26] and cyclohexane + *p*-xylene,[27] experimental excess Gibbs free energies are available in the chemical literature at or near 25°C. Excess Gibbs free energies of the remaining five systems were estimated *via* the Scatchard–Hildebrand solubility parameter model

$$\bar{G}_{12}^{ex} = \phi_1^0\phi_2^0(X_1^0\bar{V}_1 + X_2^0\bar{V}_2)(\delta_1 - \delta_2)^2 \tag{2}$$

where $\delta_i$ is the solubility parameter of component $i$. Table 3 lists numerical values of solubility parameters, molar volumes and surface areas used in the NIBS predictions. Surface areas of the individual molecules are taken from tabulated values presented in previous reports.[28–31] In all cases, the surface areas exclude solvent molecules which may be located within the solvation sphere surrounding the solute molecule.

Inspection of Table 2 reveals that Eq. (XA), based on surface areas as weighting factors for the excess Gibbs free energies relative to Raoult's law, is found to be the "best" predictive expression with an overall average (rms) deviation of 3.8% and a maximum error for a single data point of 16%. Deviations between observed and predicted solubilities for anthracene are larger than experimental uncertainties. It must be remembered, however, that three measured values are needed for each NIBS prediction. Anthracene solubility in each pure solvent was reproducible to within 1%

**Table 2** Summarized comparison between experimental anthracene solubilities and values predicted from the NIBS equations.

| *Binary solvent system* | *% Deviations of Calculated Values*[a] | | | | |
|---|---|---|---|---|---|
| | *(XX)* | *(XV)* | *(XA)* | *(VV)* | *(VA)* |
| *n*-Hexane + *p*-Xylene | −7.9 | −8.2 | −2.0 | −8.2 | −2.0 |
| *n*-Heptane + *p*-Xylene | +0.7 | −4.0 | +1.2 | −3.9 | +1.4 |
| *n*-Octane + *p*-Xylene | +2.0 | −5.9 | −1.3 | −5.9 | −1.2 |
| Cyclohexane + *p*-Xylene | −12.7 | −5.3 | 0.6 | −5.3 | 0.6 |
| Methylcyclohexane + *p*-Xylene | −10.0 | −9.9 | −5.1 | −9.9 | −5.1 |
| Isooctane + *p*-Xylene | +10.6 | 0.6 | +13.3 | 0.6 | +13.5 |
| Methylcyclohexane + Benzene | +2.7 | −4.7 | 2.9 | −4.2 | 3.5 |
| *n*-Octane + Benzene | +12.7 | 2.2 | +4.0 | 1.4 | +5.2 |

[a] Deviation (%) = $(100/N^{1/2})\{\sum[\ln(X_3^{cal}/X_3^{exp})]^2\}^{1/2}$; an algebraic sign indicates that all deviations were of the same sign.

**Table 3** Solute and solvent properties used in the NIBS predictions.

| *Component* | $\bar{V}_i$, *cm*$^3$*/mole* | $\bar{A}_i$, Å$^2$*/mole* | $\delta_i$, *cal*$^{1/2}$ *cm*$^{-3/2,a}$ |
|---|---|---|---|
| *n*-Hexane | 131.51 | 142.1 | 7.27 |
| *n*-Heptane | 147.48 | 160.3 | 7.50 |
| *n*-Octane | 163.46 | 178.4 | 7.54 |
| Cyclohexane | 108.76 | 120.8 | |
| Methylcyclohexane | 128.32 | 137.7 | 7.83 |
| Isooctane | 166.09 | 163.1 | 6.86 |
| Benzene | 89.41 | 109.5 | |
| *p*-Xylene | 123.93 | 150.3 | 8.83 |
| Anthracene | 150.00 | 202.2 | $a_3^{\text{solid}} = 0.01049$ |

[a] Solubility parameters are taken from Hoy[34], except for methycyclohexane which was calculated from data in Majer *et al.*[35]

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and experimental $\bar{G}_{12}^{\text{ex}}$ values, which are available for only three of the binary solvent systems, are believed to be accurate to at least ±6 cal/mole. Uncertainties of the estimated $\bar{G}_{12}^{\text{ex}}$ values may even be much larger. Ratios of $\Gamma_3/(X_1^0\Gamma_1 + X_2^0\Gamma_2)$ greater than unity magnify the effect that errors in the unmixing term has on the solubility predictions. A 6 cal/mole error in $\Gamma_3(X_1^0\Gamma_1 + X_2^0\Gamma_2)^{-1}\bar{G}_{12}^{\text{ex}}$ corresponds to an error of 1% in the predicted value. Based on these observations, "uncertainties" in the NIBS predictions are estimated to be on the order of 2-3%, which in part explains deviations between observed and predicted values. The much larger deviations noted in the isooctane + *p*-xylene are probably attributed to errors in the $\bar{G}_{12}^{\text{ex}}$ values. For the isooctane + *p*-xylene system the excess Gibbs free energies were not available in the chemical literature and thus were estimated *via* Eq. (2).

An important consequence of this research involves earlier contentions that the failure of Eq. (1) may be taken as an indication of specific solute-solvent or solvent-solvent interactions. While this concept is relatively straighforward in principle, its practical applications can be complicated by the various weighting factor approximations. For example, does the failure of Eqs (XV) and (VV) to predict anthracene solubilities in binary mixtures containing *p*-xylene indicate specific solute-solvent ($\pi$–$\pi$) interactions, or does the success of Eq. (XA) (and (VA)) indicate that surface areas provide a better approximation of weighting factors in systems containing both a planar aromatic hydrocarbon solute and solvent molecule.

Price and Stone[32] have recently suggested that benzene forms weak van der Waals complexes with anthracene and perylene. Using quantum mechanical calculations, the authors located minima in the electrostatic energy surfaces. Electrostatic interactions favored two types of stuctures for the anthracene-benzene complex. The first set corresponded to approximately displaced parallel plate structures, with the edge of the benzene molecule roughly parallel to the long axis of anthracene. T-shaped complexes represented the second set of structures and the edge of the benzene molecule points to either the central or end ring of anthracene. A possible anthracene-xylene complex can be argued on the basis of structural similarities between benzene and *p*-xylene.

Accepting for the moment that anthracene does form a molecular complex with *p*-xylene, the association constant for this *presumed* complex can be calculated from the Extended NIBS model[6,33]

$$A + C \rightleftharpoons AC \qquad K^{\phi}_{AC} = \hat{\phi}_{AC}/(\hat{\phi}_{A_1}\hat{\phi}_{C_1})$$

$$\ln \phi_A^{\text{sat}} = \phi_B^0 \ln(\phi_A^{\text{sat}})_B + \phi_C^0 \ln(\phi_A^{\text{sat}})_C - \phi_C^0 \ln[1 + \bar{V}_A K^{\phi}_{AC}/(\bar{V}_A + \bar{V}_C)]$$

$$+ \ln[1 + \bar{V}_A \phi_C^0 K^{\phi}_{AC}/(\bar{V}_A + \bar{V}_C)] + \frac{\bar{V}_A \bar{G}^{\text{fh}}_{BC}}{RT(X_B^0 \bar{V}_B + X_C^0 \bar{V}_C)}$$

and the solute solubility (component A) as a function of complexing solvent concentration (component C). The numerical value of the calculated anthracene-xylene equilibrium constant, $K^{\phi}_{AC} \approx 1$–$2$ is quite small and would suggest at best only a very weak molecular complex. Readers are reminded that the calculation of an equilibrium constant for a *presumed* anthracene-xylene complex does not imply that the authors believe that such a complex exist in solution. The presence of molecular complexes should be supported by a number of independent measurements involving spectroscopy, calorimetry, *etc.* Irrespective of whether complexation does occur in these systems, results of the present study show that the best expressions for predicting anthracene solubilities in binary alkane + *p*-xylene solvent mixtures approximate weighting factors with molecular surface areas.

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### *Acknowledgements*

Acknowledgement is made to the Donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research.

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