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Solubility of Anthracene in Ternary 2-Butoxyethanol + Alkane + Propanol Solvent Mixtures

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Experimental solubilities are reported for anthracene dissolved in ternary 2-butoxyethanol + cyclohexane + 1-propanol, 2-butoxyethanol + cyclohexane + 2-propanol, 2-butoxyethanol + heptane + 1-propanol, and 2-butoxyethanol + heptane + 2-propanol solvent mixtures at 298.15 K. Nineteen compositions were studied for each of the four solvent systems. Results of these measurements, along with published anthracene solubility data in 20 additional ternary two alkane + alcohol and alkane + two alcohol solvent systems, are used to test the predictive ability of the combined nearly ideal multiple solvent (NIMS)/Redlich−Kister and combined NIMS/BAB equations. Computations showed that the combined NIMS/Redlich−Kister equation predicted the experimental solubility data to within an overall average absolute deviation of about 1.4% for the 24 systems considered in the present study. A slightly larger deviation of about 1.6% was noted in the case of the combined NIMS/BAB equation.

Introduction

Solid−liquid equilibrium data of organic nonelectrolyte systems are becoming increasingly important in the petroleum industry, particularly in light of present trends toward heavier feedstocks and the known carcinogenicity/mutagenicity of many of the larger polycyclic aromatic compounds. Solubility data for a number of polycyclic aromatic hydrocarbons (i.e., anthracene and pyrene) and heteroatom polynuclear aromatics (i.e., carbazole, dibenzothiophene, and xanthene) have been published in the recent chemical literature. For a listing of references, see Acree (1994, 1995a,b). 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 group contribution methods and semiempirical equations to predict desired quantities from either pure component properties or measured binary data. In earlier studies we have used the binary solvent reduction of a predictive expression derived from a combined two- and three-body interactional mixing model as a mathematical representation for describing how the measured isothermal solubility of a crystalline solute varies with binary solvent composition. The binary reduction, referred to as the combined nearly ideal multiple solvent (NIMS)/Redlich−Kister equation, was found to accurately describe the observed solubility behavior in a large number of different binary solvent systems (Acree, 1992; Acree and Zvaigzne, 1991; Acree et al., 1991). Our mathematical representation, when extended to ternary solvent mixtures, was recently found to provide reasonably accurate predictions for the mole fraction solubility of anthracene, $x_A^{\text{sat.}}$, in 8 different ternary two alkane + alcohol (Deng and Acree, 1998a; Deng et al., 1999b) and 12 different ternary alkane + two alcohol (Deng and Acree, 1998b; Deng et al., 1998, 1999a) solvent mixtures

$$\ln x_A^{\text{sat.}} = x_B^\circ \ln (x_A^{\text{sat.}})_B + x_C^\circ \ln (x_A^{\text{sat.}})_C + x_D^\circ \ln (x_A^{\text{sat.}})_D + x_B^\circ x_C^\circ \sum_{i=0}^{r} S_{i,BC}(x_B^\circ - x_C^\circ)^i + x_B^\circ x_D^\circ \sum_{j=0}^{s} S_{j,BD}(x_B^\circ - x_D^\circ)^j + x_C^\circ x_D^\circ \sum_{k=0}^{t} S_{k,CD}(x_C^\circ - x_D^\circ)^k \quad (1)$$

using curve-fit parameters ($S_{i,BC}$, $S_{j,BD}$, and $S_{k,CD}$) deduced from the measured anthracene solubility data in the three contributing subbinary solvent systems. In the above expression x_B°, x_C°, and x_D° denote the initial mole fraction compositions of the ternary solvent mixture calculated in the absence of the solute. In keeping with our past terminology, eq 1 will be referred to hereafter as the ternary solvent form of the more general combined NIMS/Redlich−Kister model.

In the present investigation we report the solubility of anthracene in four ternary 2-butoxyethanol + alkane + propanol solvent mixtures. These measurements were performed so that we could better assess the predictive accuracy of eq 1. Anthracene is considerably more soluble in 2-butoxyethanol than in alkane (cyclohexane and heptane) and alcohol (1-propanol and 2-propanol) solvents. The four ternary 2-butoxyethanol + alkane + propanol solvent systems cover up to a 9-fold range in anthracene mole fraction solubility. In comparison, the 20 ternary systems studied previously covered a much smaller 4-fold range in anthracene mole fraction solubility.

Experimental Methods

Anthracene (Acros, 99.9+%) was recrystallized three times from 2-propanone. 1-Propanol (Aldrich, 99+%, anhydrous), 2-propanol (Aldrich, 99+%, anhydrous), cyclohexane (Aldrich, HPLC, 99.9+%), heptane (Aldrich, HPLC, 99+%), and 2-butoxyethanol (Acros, 99+%) were stored over molecular sieves and distilled shortly before use. Gas chromatographic analysis showed solvent purities to be 99.7 mol % or better. Ternary solvent mixtures were pre-

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pared by mass so that compositions could be calculated to 0.0001 mole fraction. The methods of sample equilibration and spectrophotometric analysis are discussed in an earlier paper (Powell et al., 1997). Experimental anthracene solubilities in the four 2-butoxyethanol + alkane + propanol solvent mixtures are listed in Table 1. 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

Conceptually, eq 1 traces back to when Acree and Bertrand (1981) employed the NIBS model to estimate the solubility of benzoic acid in ternary solvent mixtures. The authors derived expressions based upon the assumption that the carboxylic acid solute existed in solution entirely as monomers or completely in dimeric form. The assumptions represented the two limiting conditions. For molecules having identical molar volumes, the predictive expression derived by the authors can be written as

$$\ln x_A^{\text{sat.}} = x_B^\circ \ln (x_A^{\text{sat.}})_B + x_C^\circ \ln (x_A^{\text{sat.}})_C + x_D^\circ \ln (x_A^{\text{sat.}})_D + G^E_{BCD}(RT)^{-1} \quad (2)$$

a weighted mole fraction average of the logarithmic solute solubilities in the three pure solvents plus a term containing the excess Gibbs free energy of the ternary solvent mixtures. Equation 2 is derived for solutes having very limited saturation solubilities.

Thermodynamic properties of ternary mixtures were relatively scarce in 1981, and the required G^E_{BCD} values had to be estimated from available binary vapor−liquid equilibria (VLE) data. Several predictive models had been suggested for estimating ternary thermodynamic and physical properties from measured binary data. Equation 1 can be derived by substituting the Redlich−Kister prediction for

$$G^E_{BCD} = x_B^\circ x_C^\circ \sum_{i=0}^{r} G_{i,BC}(x_B^\circ - x_C^\circ)^i + x_B^\circ x_D^\circ \sum_{j=0}^{s} G_{j,BD}(x_B^\circ - x_D^\circ)^j + x_C^\circ x_D^\circ \sum_{k=0}^{t} G_{k,CD}(x_C^\circ - x_D^\circ)^k \quad (3)$$

into eq 2. The various $G_{i,BC}$, $G_{j,BD}$, and $G_{k,CD}$ values represent coefficients deduced from a regressional analysis of experimental binary VLE data. Our approach differs slightly in application in that we now prefer to determine the Redlich−Kister coefficients from measured solute solubilities in the three contributing subbinary solvent mixtures, rather than from available VLE data. To indicate this practice, we have denoted the curve-fit coefficients in eq 1 as $S_{i,BC}$, $S_{i,BC}$, and $S_{i,CD}$. The binary reduction of eq 1 has been used as a mathematical representation of experimental isothermal mole fraction solubility data for solutes dissolved in binary solvent mixtures. In the case of solutes dissolved in binary aqueous−organic solvent mixtures, the experimental solubility data were represented by a modified form of eq 1 which contained volume fraction compositions of the various solvent components rather than mole fractions (Jouyban-Gharamaleki and Acree, 1998; Jouyban-Gharamaleki et al., 1998). The modified form is derivable from the general NIBS model by approximating the weighting factors with molar volumes. Equation 1 assumes that the weighting factors of all components are equal.

Table 1. Experimental Mole Fraction Solubilities of Anthracene ($x_A^{\text{sat.}}$) in Ternary 2-Butoxyethanol (B) + Alkane (C) + Propanol (D) Solvent Mixtures at 298.15 K

x_B°	x_C°	$x_A^{\text{sat.}}$	x_B°	x_C°	$x_A^{\text{sat.}}$
2-Butoxyethanol (B) + Cyclohexane (C) + 1-Propanol (D)					
0.2553	0.3071	0.001 884	0.0983	0.1162	0.001 007
0.1209	0.6708	0.001 931	0.6117	0.1596	0.002 790
0.1765	0.2124	0.001 402	0.4030	0.2454	0.002 262
0.1946	0.4688	0.001 936	0.0645	0.1545	0.000 957
0.5976	0.1057	0.002 560	0.0758	0.6533	0.001 791
0.6221	0.2189	0.003 045	0.1281	0.0793	0.001 038
0.1638	0.6923	0.002 182	0.0692	0.3297	0.001 272
0.0721	0.4298	0.001 487	0.2874	0.0866	0.001 531
0.3389	0.5103	0.002 520	0.3752	0.0952	0.001 855
0.4313	0.4151	0.002 801			
2-Butoxyethanol (B) + Cyclohexane (C) + 2-Propanol (D)					
0.2543	0.3097	0.001 786	0.0980	0.1191	0.000 846
0.1193	0.6769	0.001 912	0.6122	0.1608	0.002 776
0.1768	0.2147	0.001 283	0.4048	0.2476	0.002 169
0.1954	0.4718	0.001 899	0.0651	0.1560	0.000 817
0.6002	0.1050	0.002 560	0.0780	0.6558	0.001 723
0.6257	0.2178	0.002 977	0.1322	0.0805	0.000 874
0.1632	0.6909	0.002 115	0.0704	0.3352	0.001 153
0.0745	0.4356	0.001 342	0.2889	0.0898	0.001 360
0.3403	0.5148	0.002 607	0.3828	0.0938	0.001 676
0.4308	0.4198	0.002 712			
2-Butoxyethanol (B) + Heptane (C) + 1-Propanol (D)					
0.2770	0.2433	0.001 844	0.1003	0.0882	0.001 013
0.1463	0.5948	0.001 931	0.6392	0.1221	0.002 888
0.1856	0.1644	0.001 426	0.4298	0.1908	0.002 221
0.2274	0.3881	0.001 932	0.0687	0.1174	0.000 945
0.6136	0.0798	0.002 601	0.0962	0.5804	0.001 727
0.6615	0.1688	0.003 033	0.1336	0.0594	0.001 061
0.2017	0.6251	0.002 182	0.0768	0.2680	0.001 261
0.0822	0.3568	0.001 378	0.2925	0.0670	0.001 508
0.3921	0.4377	0.002 591	0.3893	0.0697	0.001 845
0.4854	0.3442	0.002 769			
2-Butoxyethanol (B) + Heptane (C) + 2-Propanol (D)					
0.2779	0.2506	0.001 699	0.1035	0.0933	0.000 853
0.1451	0.6020	0.001 867	0.6409	0.1245	0.002 783
0.1894	0.1686	0.001 255	0.4340	0.1941	0.002 170
0.2240	0.3978	0.001 817	0.0686	0.1211	0.000 803
0.6184	0.0806	0.002 595	0.0967	0.5846	0.001 634
0.6671	0.1708	0.002 968	0.1353	0.0600	0.000 872
0.2021	0.6202	0.002 087	0.0785	0.2694	0.001 085
0.0818	0.3594	0.001 217	0.2971	0.0662	0.001 334
0.3921	0.4316	0.002 482	0.3943	0.0700	0.001 704
0.4800	0.3448	0.002 665			

Careful inspection of eq 1 requires that one must parametrize the measured binary solvent solubility data in the specific form of

$$\ln x_A^{\text{sat.}} = x_B^\circ \ln (x_A^{\text{sat.}})_B + x_C^\circ \ln (x_A^{\text{sat.}})_C + x_B^\circ x_C^\circ \sum_{i=0}^{n} S_{i,BC}(x_B^\circ - x_C^\circ)^i \quad (4)$$

as the actual numerical values of the $S_{i,BC}$ coefficients are needed in the calculation. This requirement presents no problems in the present study as the coefficients of eq 4 were given when we communicated the binary solvent solubility data. Not all researchers parametrize measured solubility data in accordance with eq 4. For example, in the pharmaceutical industry isothermal solubility data may be expressed in terms of the extended Hildebrand solubility parameter approach (Barra et al., 1997; Martin et al., 1980, 1982), the double log−log model (Barzegar-Jalali and Hanaee, 1994), or the modified Wilson model (Jouyban-Gharamaleki, 1998) or as a power series expansion in mole fraction composition of one of the binary solvent components. Solubility data for select crystalline polycyclic aromatic hydrocarbons dissolved in binary aqueous−organic

Table 2. Summarized Comparison between Experimental Anthracene Solubilities and Predicted Values Based upon the Combined NIMS/Redlich−Kister and Combined NIMS/BAB Equations

ternary solvent system	percent deviations[a]	
	NIMS/Redlich−Kister	NIMS/BAB
2-butoxyethanol + cyclohexane + 1-propanol	1.63	2.29
2-butoxyethanol + cyclohexane + 2-propanol	1.58	3.01
2-butoxyethanol + heptane + 1-propanol	1.48	1.13
2-butoxyethanol + heptane + 2-propanol	1.25	2.29
1-propanol + 1-butanol + cyclohexane	1.45	1.66
1-propanol + 2-butanol + cyclohexane	1.76	1.93
2-propanol + 1-butanol + cyclohexane	1.70	2.04
2-propanol + 2-butanol + cyclohexane	1.57	1.74
1-propanol + 1-butanol + heptane	1.30	1.30
1-propanol + 2-butanol + heptane	0.96	1.16
2-propanol + 1-butanol + heptane	1.64	1.64
2-propanol + 2-butanol + heptane	1.69	1.25
1-propanol + 1-butanol + 2,2,4-trimethylpentane	0.77	0.80
1-propanol + 2-butanol + 2,2,4-trimethylpentane	0.52	0.72
2-propanol + 1-butanol + 2,2,4-trimethylpentane	1.11	0.94
2-propanol + 2-butanol + 2,2,4-trimethylpentane	1.27	1.06
1-propanol + 2,2,4-trimethylpentane + cyclohexane	1.60	1.31
2-propanol + 2,2,4-trimethylpentane + cyclohexane	1.40	1.87
1-butanol + 2,2,4-trimethylpentane + cyclohexane	1.70	1.63
2-butanol + 2,2,4-trimethylpentane + cyclohexane	1.71	1.73
1-propanol + heptane + cyclohexane	1.55	1.92
2-propanol + heptane + cyclohexane	0.92	1.62
1-butanol + heptane + cyclohexane	1.11	1.20
2-butanol + heptane + cyclohexane	1.58	1.60
OVERALL AVERAGE ABSOLUTE DEVIATION	1.39	1.58

[a] Deviation (%) = $(100/19)\sum|[(x_A^{sat.})^{calc} - (x_A^{sat.})^{exp}]/(x_A^{sat.})^{exp}|$.

solvent mixtures were described using the Margules equation in a recently published paper (Fan and Jafvert, 1997) appearing in an environmental science journal.

We note that the aforementioned solubility study of Acree and Bertrand (1981) contained provisions for mathematical representations other than the Redlich−Kister equation. There is no requirement that the ternary G^E_{BCD} value in eq 2 be estimated with the Redlich−Kister equation. In fact, Acree and Bertrand used the BAB equation to generate the excess Gibbs energy of the ternary solvent in their benzoic acid solubility study. The BAB equation combines binary G^E_{IJ} values at specified solvent concentrations

$$G^E_{BCD} = (x_B^\circ + x_C^\circ)^2 (G^E_{BC})^* + (x_B^\circ + x_D^\circ)^2 (G^E_{BD})^* + (x_C^\circ + x_D^\circ)^2 (G^E_{CD})^* \quad (5)$$

rather than using coefficients of a particular mathematical representation. The excess Gibbs energy of the IJ binary solvent mixture, $(G^E_{IJ})^*$, is calculated at a mole fraction composition of $x_I^* = x_I^\circ/(x_I^\circ + x_J^\circ)$. The BAB equation is described in greater detail elsewhere (Bertrand et al., 1983; Acree and Bertrand, 1983). As in the case of eq 1, we will determine the needed $(G^E_{IJ})^*$ values from measured solubility data in the three binary contributing subbinary solvent systems

$$(G^E_{IJ})^*(RT)^{-1} = \ln x_A^{sat.}(\text{at } x_I^*) - x_I^* \ln (x_A^{sat.})_I - x_J^* \ln (x_A^{sat.})_J \quad (6)$$

when using the combined NIMS/BAB equation to predict anthracene solubilities in ternary solvent mixtures. Any mathematical representation can be used for describing how $\ln x_A^{sat.}$ varies with binary solvent composition.

The predictive abilities of the combined NIMS/Redlich−Kister and Combined NIMS/BAB equations are summarized in Table 2 for anthracene dissolved in 24 different solvent systems. Experimental data for the first four solvent systems were measured as part of the present study. For convenience we have listed in Table 3 the various S_i curve-fit coefficients needed in eq 1 to predict the solubility of anthracene in the four ternary 2-butoxyethanol + alkane + propanol solvent mixtures. The curve-fit parameters, along with the measured solubilities in 1-propanol ($x_A^{sat.} = 0.000\,591$), 2-propanol ($x_A^{sat.} = 0.000\,411$), cyclohexane ($x_A^{sat.} = 0.001\,553$), heptane ($x_A^{sat.} = 0.001\,571$), and 2-butoxyethanol ($x_A^{sat.} = 0.003\,785$), were taken from

Table 3. Combined NIBS/Redlich−Kister Parameters Calculated from Anthracene Solubilities in the Subbinary Solvent Systems

solvent (B) + solvent (C)	S_i[a]
cyclohexane (B) + 1-propanol (C)	1.121 0.040 0.256
2-butoxyethanol (B) + 1-propanol (C)	1.222 −0.572 0.255
2-butoxyethanol (B) + heptane (C)	0.928 −0.488 0.123
heptane (B) + 1-propanol (C)	1.098 −0.106 0.324
2-butoxyethanol (B) + 2-propanol (C)	1.550 −0.790 0.726
cyclohexane (B) + 2-propanol (C)	1.589 −0.143 0.248
heptane (B) + 2-propanol (C)	1.491 −0.587 0.566
2-butoxyethanol (B) + cyclohexane (C)	1.081 −0.863 0.565

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

our earlier publications (Acree et al., 1994; Hernández et al., 1997; McHale et al., 1996; Zvaigzne et al., 1993). Experimental anthracene solubilities in the 8 ternary two alkane + alcohol and 12 ternary alkane + two alcohol solvent mixtures were published elsewhere (Deng and Acree, 1998a,b; Deng et al., 1998, 1999a,b). The S_i curve-fit parameters for the respective contributing subbinary solvent systems are also listed in the papers containing the ternary solvent solubility data. Examination of the numerical entries in Table 2 reveals that both models provide very reasonable predictions for the solubility behavior of anthracene. The overall average absolute deviation between experimental and predicted mole fraction solubilities is approximately 1.4% and 1.60% for the combined NIMS/Redlich−Kister and combined NIMS/BAB equations, respectively. Deviations are comparable in magnitude to the ±1.5% experimental uncertainty associated with each measured mole fraction solubility. For many of the systems considered both models gave comparable predicted values. The major exceptions are those systems which contain 2-butoxyethanol. The 2-butoxyethanol systems are highly nonideal, and the "excess logarithmic mole fraction solubility" of several of the contributing subbinary solvent systems, defined as $\ln x_A^{\text{sat.}}(\text{at } x_I^*) - x_I^* \ln(x_A^{\text{sat.}})_I - x_J^* \ln(x_A^{\text{sat.}})_J$, is highly skewed toward one of the binary solvent components. The skew is what leads to the differences in predicted values for the two models. The combined NIMS/Redlich−Kister and combined NIMS/BAB equations would have given identical predicted values had the excess logarithmic mole fraction solubility of the contributing subbinary solvent systems been symmetrical.

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