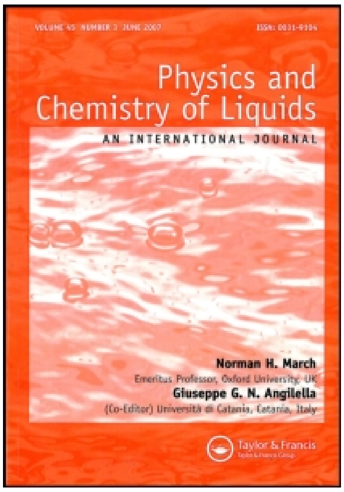

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Mathematical Representation of Thermodynamic Properties. Carbazole Solubilities in Binary Alkane Dibutyl Ether and Alkane Tetrahydropyran Solvent Mixtures

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MATHEMATICAL REPRESENTATION OF THERMODYNAMIC PROPERTIES. CARBAZOLE SOLUBILITIES IN BINARY ALKANE + DIBUTYL ETHER AND ALKANE + TETRAHYDROPYRAN SOLVENT MIXTURES

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Experimental solubilities are reported for carbazole dissolved in binary mixtures containing tetrahydropyran with *n*-hexane, *n*-heptane, clyclohexane, isooctane, *n*-hexadecane and *t*-butylcyclohexane at 25°C. Results of these measurements, along with published carbazole solubilities in ten alkane + dibutyl ether mixtures, are used to test two mathematical representations based upon the combined Nearly Ideal Binary Solvent (NIBS)/Redlich–Kister equations and Modified Wilson model. For the systems studied, the Modified Wilson equation is found to be the better two-parameter mathematical representation with deviations between experimental and back-calculated values being on the order of $\pm 3\%$ or less. The NIBS/Redlich–Kister representation requires up to four adjustable "curve-fit" parameters to describe the solubility data.

KEY WORDS: Carbazole solubilities, mathematical representation, binary solvent systems, tetrahydropyran-alkane mixtures, dibutyl ether-alkane mixtures.

INTRODUCTION

For many years the chemical industry has recognized the importance of thermodynamic and physical properties in design calculations involving chemical separations, fluid flow and heat transfer. Development of flow calorimeters, continuous dilution dilatometers and vibrating-tube densimeters has enabled the experimental determination of excess enthalpies, heat capacities and volumes of nonelectrolyte liquid mixtures with convenience and accuracy. The use of continuous dilution methods, combined with automated chromatographic head-space sampling devices, has reduced the experimental time needed for the conventional vapor pressure and vapor-liquid equilibrium measurements. However, even with today's modern instrumentation, experimental measurments of thermodynamic properties become progressively more difficult and time-consuming with each additional component beyond binary mixtures.

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In the chemical literature, properties for binary mixtures are relatively abundant as scientific organizations have begun to compile and publish measured values in data table format. Properties for ternary systemes are scarce and properties for higher-order multicomponent systems are virtually non-existent. During the past fifty years researchers have turned to predictive methods as a way to generate desired quantities from pure component physical properties, measured binary data and/or structural information. Derived expressions generally will provide very reasonable estimates of integral excess Gibbs free energies, excess enthalpies and excess volumes for nonelectrolyte multicomponent systems containing only nonspecific interactions (noncomplexing systems) and at concentrations far removed from infinite dilution.[1-4] Near infinite dilution, many of the solution models begin to fail, particularly in systems which have strong solute-solvent complexation or solute self-association. Inherent in these computations is the additional requirement that one be able to express mathematically how the measured binary data varies with mixture composition.

The Redlich–Kister equation,[5] along with several other suggested power series and/or polynomial expansions,[6-10] have provided convenient mathematical representations for volumetric, enthalpic and excess free energy data. There are numerous thermodynamic and physical properties, however, for which standard mathematical representational forms do not exist. To address this problem, we recently suggested two possible equations for describing experimental solute solubility data in binary solvent mixtures based on either the Nearly Ideal Binary Solvent (NIBS) model

$$\ln X_A^{\mathrm{sat}} = X_B^0 \ln(X_A^{\mathrm{sat}})_B + X_C^0 \ln(X_A^{\mathrm{sat}})_C + X_B^0 X_C^0 \sum_{i=0}^{r} S_i (X_B^0 - X_C^0)^i \tag{1}$$

or Modified Wilson equation

$$\ln(a_A^{\mathrm{solid}}/X_A^{\mathrm{sat}}) = 1 - \frac{X_B^0\{1 - \ln[a_A^{\mathrm{solid}}/(X_A^{\mathrm{sat}})_B]\}}{X_B^0 + X_C^0 \Lambda_{BC}^{\mathrm{adj}}} - \frac{X_C^0\{1 - \ln[a_A^{\mathrm{solid}}/(X_A^{\mathrm{sat}})_C]\}}{X_B^0 \Lambda_{CB}^{\mathrm{adj}} + X_C^0} \tag{2}$$

where the various S_i and $\Lambda_{ij}^{\mathrm{adj}}$ "curve-fit" parameters are determined *via* least squares analysis.[11] Symbols used in Eqs. (1) and (2) are defined in the glossary at the end of the manuscript. Our preliminary calculations involving anthracene dissolved in six binary alkane + 1-chlorobutane solvent mixtures showed that both expressions could describe the observed 5-fold range in mole fraction solubilities to within the experimental uncertainty of ±1.5%. Further studies are needed on systems covering much broader solubility ranges, though, in order to properly assess the applications and limitations of Eqs. (1) and (2). For this reason we have measured carbazole solubilities in binary solvent mixtures containing tetrahydropyran with cyclohexane, *n*-hexane, *n*-heptane, isooctane, *t*-butylcyclohexane and *n*-hexadecane. These systems cover up to a 340-fold solubility range, and when combined with previously reported data for carbazole in ten alkane + dibutyl ether mixtures (up to a 40-fold range),[12-14]

Table 1 Experimental mole fraction solubilities of carbazole in several binary solvent mixtures at 25.0°C.

Solvent (B) + Solvent (C)	X_C^0	X_A^{sat}
n-Hexane + Tetrahydropyran	0.0000	0.000139
	0.1442	0.002243
	0.2555	0.005188
	0.3674	0.008676
	0.4701	0.01259
	0.5741	0.01761
	0.6684	0.02257
	0.8405	0.03180
	0.9262	0.03763
	1.0000	0.04284
Cyclohexane + Tetrahydropyran	0.0000	0.000183
	0.1192	0.001509
	0.2183	0.003271
	0.3270	0.006033
	0.3861	0.007828
	0.5230	0.01325
	0.6259	0.01832
	0.7204	0.02339
	0.8172	0.03082
	0.9079	0.03761
	1.0000	0.04284
n-Heptane + Tetrahydropyran	0.0000	0.000173
	0.0480	0.000496
	0.1188	0.001142
	0.2475	0.002993
	0.3656	0.005155
	0.5020	0.009344
	0.5988	0.01381
	0.7161	0.02081
	0.8172	0.02821
	0.9119	0.03608
	1.0000	0.04284
Isooctane + Tetrahydropyran	0.0000	0.000126
	0.1394	0.001041
	0.2076	0.001652
	0.3032	0.002863
	0.3949	0.004538
	0.5021	0.007441
	0.6073	0.01138
	0.6992	0.01602
	0.8007	0.02297
	0.9032	0.03210
	1.0000	0.04282
t-Butylcyclohexane + Tetrahydropyran	0.0000	0.000250
	0.0889	0.001087
	0.1997	0.002499
	0.3093	0.004449
	0.4025	0.006748
	0.4873	0.009092
	0.6116	0.01419
	0.7072	0.01922

(Continued on next page)

Table 1 (*Continued*)

Solvent (B) + Solvent (C)	X_C^0	X_A^{sat}
	0.8036	0.02549
	0.9041	0.03361
	1.0000	0.04284
n-Hexadecane + Tetrahydropyran	0.0000	0.000414
	0.0745	0.000985
	0.1539	0.001723
	0.2686	0.003019
	0.3531	0.004235
	0.4315	0.005579
	0.5332	0.007994
	0.6396	0.01215
	0.7495	0.01812
	0.8487	0.02473
	0.9411	0.03439
	1.0000	0.04284

should provide a clearer indication of each equation's ability to mathematically represent experimental data.

MATERIALS AND METHODS

Carbazole (Aldrich 99%) was recrystallized several times from absolute ethanol, giving a melting point temperature of 246.5 ± 0.5°C (literature value 247–248°C[15]). Cyclohexane (Aldrich HPLC grade), *n*-hexane (Aldrich 99%), *n*-heptane (Aldrich HPLC grade), isooctane (Aldrich HPLC grade), *t*-butylcyclohexane (Aldrich 99+%, *n*-hexadecane (Aldrich 99%), and tetrahydropyran (Aldrich 99% anhydrous) were stored over molecular sieves to remove trace amounts of water. Binary solvent mixtures were prepared by weight so that solvent compositions could be calculated to 0.0001 mole fraction.

Excess carbazole and solvent were placed in amber glass bottles and allowed to equilibrate in a constant temperature shaker bath at 25.0 ± 0.1°C for several days. The attainment of equilibrium was verified by repetitive measurements after several additional days and in some cases by approaching equilibrium from supersaturation by pre-equilibrating the solution at a higher temperature. Aliquots of saturated carbazole solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with methanol (carbon tetrachloride in the case of *n*-hexadecane). Concentrations were determined spectrophotometrically at 292 nm on a Bausch and Lomb Spectronic 2000. At this particular wavelength, two to four serial dilutions were necessary in order to get the more concentrated carbazole solutions to fall within the linear concentration versus absorbance region. Experimental solubilities of carbazole in the six binary solvent systems studied are listed in Table 1. Numerical values represent the average of between 6 and 8 independent determinations. Measurements were reproducible to

Table 2 Mathematical representation of carbazole solubilities in several binary alkane (B) + dibutyl ether (C) and alkane (B) + tetrahydropyran (C) solvent mixtures.

Binary solvent system	*Eq. (1)*		*Eq. (1)*		*Eq. (2)*	
	S_i^{a}	*% Dev.*[b]	S_i^{a}	*% Dev.*[b]	$\Lambda_{ij}^{adj,c}$	*% Dev.*[b]
t-Butylcyclohexane + Tetrahydropyran	5.473 4.931	17.8	4.250 2.901 4.024 3.878	2.6	1.151 0.116	1.5
n-Hexane + Tetrahydropyran	8.415 6.558	19.7	6.951 5.102 5.739 4.806	1.9	2.280 0.0560	1.1
n-Hexadecane + Tetrahydropyran	2.971 3.216	11.6	2.103 2.001 2.776 1.992	1.3	0.650 0.219	3.2
Cyclohexane + Tetrahydropyran	7.153 5.214	18.4	5.901 4.004 4.265 3.495	3.8	1.800 0.0900	1.6
n-Heptane + Tetrahydropyran	6.863 6.334	25.8	4.853 2.551 5.161 5.564	3.3	1.405 0.106	3.3
Isooctane + Tetrahydropyran	5.582 4.407	14.6	4.720 2.998 3.272 4.012	4.2	1.188 0.107	1.8
n-Hexane + Dibutyl ether	3.850 3.388	10.7	3.250 1.671 1.865 3.211	2.1	2.349 0.0100	2.6
n-Heptane + Dibutyl ether	3.229 2.490	5.5	2.921 1.999 1.369	2.9	2.179 0.0308	1.5
n-Octane + Dibutyl ether	3.209 2.190	7.1	2.650 2.001 2.204	1.7	2.188 0.0287	2.4
Methylcyclohexane + Dibutyl ether	4.035 3.209	10.1	3.398 2.302 2.316 1.137	1.9	2.897 0.0195	1.7
Cyclooctane + Dibutyl ether	3.829 3.105	10.9	3.200 1.998 2.074 1.856	2.7	3.113 0.0110	1.5

(*Continued on next page*)

Table 2 (*Continued*)

Binary solvent system	*Eq. (1)*		*Eq. (1)*		*Eq. (2)*	
	S_i^a	*% Dev.*[b]	S_i^a	*% Dev.*[b]	$\Lambda_{ij}^{adj,c}$	*% Dev.*[b]
n-Hexadecane + Dibutyl ether	1.618 1.092	2.7			2.630 2.985	1.6
Squalane + Dibutyl ether	0.517 0.592	1.6			1.860 4.390	1.5
t-Butylcyclohexane + Dibutyl ether	3.328 2.379	6.7	2.848 2.332 1.736	2.2	2.520 0.0260	1.8
Isooctane + Dibutyl ether	3.648 2.752	7.1	3.150 1.951 1.964 1.598	2.3	2.321 0.00833	2.0
Cytohexane + Dibutyl ether	4.286 4.438	13.7	3.615 2.750 2.387 2.067	3.7	2.926 0.000	2.2

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

[b] Deviation (%) = $(100/N) \sum |\ln(X_A^{calc}/X_A^{exp})|$

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

within ±2 for the smaller solubilities and ±4% for the more concentrated carbazole solutions. The larger experimental uncertainties are approximately twice those observed in our previous studies and result primarily from errors propagating throughout the serial dilutions.

RESULTS AND DISCUSSIONS

The ability of Eqs. (1) and (2) to mathematically represent the experimental solubility of carbazole in ten binary alkane + dibutyl ether and six alkane + tetrahydropyran solvent systems is summarized in Table 2 in the form of "curve-fit" parameters and percent deviations in back-calculated solubilities for the 2-parameter expressions. In the case of Eq. (1) the 3- and 4-parameter forms were also considered. During the course of evaluating parameters for the Modified Wilson equation, it was noted that on a Λ_{BC}^{adj} versus Λ_{CB}^{adj} versus % Deviation three-dimensional map there existed several parameter pairs which described the carbazole solubility to within the quoted uncertainty. For example, in the case of carbazole solubilities in isooctane + tetrahydropyran mixtures, the percent deviation was approximately 4.0% for $\Lambda_{BC}^{adj} = 1.300$ and $\Lambda_{CB}^{adj} = 0.14$, 2.6% for $\Lambda_{BC}^{adj} = 1.25$ and $\Lambda_{CB}^{adj} = 0.12$, and 1.8% for $\Lambda_{BC}^{adj} = 1.188$ and $\Lambda_{CB}^{adj} = 0.107$. No special attempt was made to optimize calculated Λ_{ij}^{adj} values as we wished only to learn if Eq. (2) could be used to mathematically represent experimental data in systems covering extremely large solubility ranges. Any parameter set having ±2.5% deviation was sufficient for this purpose.

The numerical value of $a_A^{\text{solid}} = 0.009354$ used in the Modified Wilson computations was calculated from

$$\ln a_A^{\text{solid}} = -\frac{\Delta \bar{H}_A^{\text{fus}}(T_{mp} - T)}{RTT_{mp}} \tag{3}$$

the molar enthalpy of fusion, $\Delta \bar{H}_A^{\text{fus}} = 27.20$ kJ/mole,[16] at the normal melting point temperature of the solute, $T_{mp} = 519.2$ K. Attempts to eliminate a_A^{solid} from the mathematical representation in favor of a simplified version $(a_A^{\text{solid}} = 1)$

$$\ln(1/X_A^{\text{sat}}) = 1 - \frac{X_B^0\{1 - \ln[1/(X_A^{\text{sat}})_B]\}}{X_B^0 + X_C^0\Lambda_{BC}^{\text{adj}}} - \frac{X_C^0\{1 - \ln[1/(X_A^{\text{sat}})_C]\}}{X_C^0 + X_B^0\Lambda_{CB}^{\text{adj}}} \tag{4}$$

proved unsuccessful.

Careful examination of Table 2 reveals that Eq. (2) provides a fairly reasonable mathematical representation of all 16 systems, which cover up to 40-fold and 340-fold solubility ranges in the case of isooctane + dibutyl ether and isooctane + tetrahydropyran, respectively. Back-calculated and experimental values generally differ by less than ±3%. Surprisingly, this simple two-parameter experession is able to imitate the sharp, pronounced solubility enhancement that occurs when both dibuty ether and tetrahydropyran are initially added to a pure alkane cosolvent. Carbazole solubilities increase between 5- and 15-fold by the time the tetrahydropyran mole fraction reaches $X_{\text{THP}}^0 = 0.15$. Based on spectroscopic studies on similar mixtures,[17-19] carbazole is expected to interact with both ethers to form a 1:1 carbazole-ether association complex. Complexation with tetrahydropyran is further suggested by the fact that the measured carbazole solubility far exceeds the activity of the solid solute, ie., $X_A^{\text{sat}} > a_A^{\text{solid}}$. The calculated activity coefficient of carbazole in pure tetrahydropyran is considerably less than unity, $\gamma_A^{\text{sat}} = a_A^{\text{solid}}/(X_A^{\text{sat}})_{\text{THP}} = 0.218$, indicating substantial negative deviations from Raoult's law. Readers should note that while Eq. (2) describes the solubility data as a whole, there are one or two individual data points within each system for which deviations may exceed ±6%. Deviations of this magnitude appear small compared against the large solubility ranges being described. In assessing the limitations of Eq. (2) one must remember that mathematical representations are not intended to replace the actual experimental solubilities, but rather are to facilitate computerized interpolations between measured data points at specific solvent compositions. With this idea in mind, Eq. (2) does mathematically describe the observed carbazole solubilities.

In comparison, the two-parameter form of Eq. (1) generally fails to describe the solubility data as the average absolute deviations are *circa* 15–25%. Many of these systems have highly skewed $\ln X_A^{\text{sat}}$ versus X_B^0 curves caused by the large initial solubility enhancement, and will necessitate expanding the Redlich–Kister power series by at least 2 (perhaps more) additional terms. Similar failures in the Redlich–Kister equation can be found in the chemical literature in the mathematical representation of excess enthalpy data for highly nonideal alcohol + hydrocarbon mixtures.[20–23] Linear least squares analysis of

$$[\ln X_A^{\text{sat}} - X_B^0 \ln(X_A^{\text{sat}})_B - X_C^0 \ln(X_A^{\text{sat}})_C]/X_B^0 X_C^0$$

versus $X_B^0 - X_C^0$ leads to abnormally large S_0 and S_1 values as the two-parameter form of Eq. (1) tries to describe the solubility behavior near the pure alkane cosolvent. Unfortunately, even with these large "curve-fit" parameters, Eq. (1) still underpredicts the initial carbazole solubilities in binary *n*-hexane + tetrahydropyran, *n*-heptane + tetrahydropyran , cyclohexane + tetrahydropyran and isooctane + tetrahydropyran mixtures by as much as 25%. At mole fraction compositions near $X_B^0 = 0.5$, Eq. (1) has overcompensated for the high initial skew and now the back-calculated solubilities are much too large. Unlike the Modified Wilson model discussed previously, Eq. (1) does contain provisions for additional parameterization. Examination of Table 2 further reveals that Eq. (1) requires 3 or 4 parameters to describe 13 of the 16 systems to within an average absolute deviation of 3.5%. Slightly larger average deviations of 3.8% and 4.2% were noted in cyclohexane + tetrahydropyran and isooctane + tetrahydropyran mixtures where the reproducibility in measured carbazole solubilities was *circa* ±4%. Again, there may be one or two individual data points within each system for which the deviation exceeds ±6%.

Readers are reminded that the 16 carbazole systems considered in the present study were judiciously selected so as to encompass extremely large solubility ranges. Many of the systems currently being studied cover less than a 10-fold mole fraction range, and can be described by either the combined NIBS/Redlich–Kister [Eq. (1)] or Modified Wilson [Eq. (2)] mathematical representations. From a computational standpoint, Eq. (1) will likely be preferred because most research groups involved in reporting thermodynamic properties have computer programs for evaluating the Redlich–Kister coefficients. In the case of the two-parameter Redlich–Kister fit, the computations require only a simple linear least squares analysis. With this idea in mind, we recommend that the future presentation of experimental isothermal solid solubility data in binary solvent mixtures include not only a tabulation of the actual observed values, but if possible, that the solubility data be mathematically represented by Eq. (1). Realizing that a single equation will not be applicable to all systems encountered, we further suggest Eq. (2) as an alternative mathematical representation for systems having large solubility ranges and/or highly asymmetrical ln X_A^{sat} versus X_B^0 curves.

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APPENDIX: GLOSSARY OF SYMBOLS

a_A^{solid}	activity of the solid solute, defined as the ratio of the fugacity of the solid to the fugacity of the pure subcooled liquid
$\Delta\bar{H}_A^{\text{fus}}$	molar enthalpy of fusion of the solute
S_i	adjustable "curve-fit" parameter in the combined NIBS/Redlich–Kister mathematical representation
X_B^0, X_C^0	mole fraction composition of the solvent mixture, calculated as if the solute were not present
X_A^{sat}	saturated mole fraction solubility of the solute
$(X_A^{\text{sat}})_i$	saturated mole fraction solubility of the solute in pure solvent component *i*
$\Lambda_{ij}^{\text{adj}}$	adjustable "curve-fit" parameter in the Modified Wilson mathematical representation
γ_A	activity coefficient of the solute