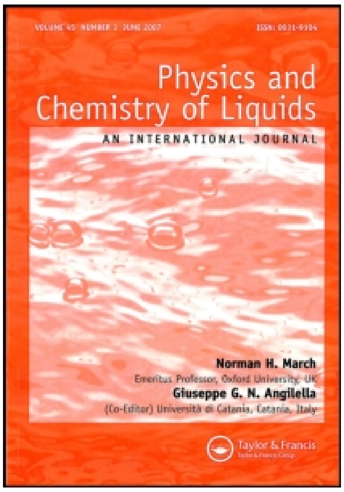

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PREDICTION AND MATHEMATICAL CORRELATION OF THE SOLUBILITY OF FLUORENE IN ALCOHOL SOLVENTS BASED UPON THE ABRAHAM GENERAL SOLVATION MODEL

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The Abraham general solvation model is used to predict the saturation solubility of crystalline nonelectrolyte solutes in organic solvents. The derived equations take the form of

$$\log(C_S/C_W) = c + rR_2 + s\pi_2^H + a\Sigma\alpha_2^H + b\Sigma\beta_2^H + vV_x$$
$$\log(C_S/C_G) = c + rR_2 + s\pi_2^H + a\Sigma\alpha_2^H + b\Sigma\beta_2^H + l\log L^{16}$$

where C_S and C_W refer to the solute solubility in the organic solvent and water, respectively, C_G is a gas phase concentration, R_2 is the solute's excess molar fraction, V_x is McGowan volume of the solute, $\Sigma\alpha_2^H$ and $\Sigma\beta_2^H$ are measures of the solute's hydrogen-bond acidity and hydrogen-bond basicity, π_2^H denotes the solute's dipolarity/polarizability descriptor, and L^{16} is the solute's gas phase dimensionless Ostwald partition coefficient into hexadecane at 298 K. The remaining symbols in the above expressions are known coefficients, which have been determined previously for a large number of gas/solvent and water/solvent systems. Computations show that the Abraham general solvation model predicts the observed solubility behavior of fluorene in 10 alcohol solvents to within an average absolute deviation of about ± 15%.

Keywords: Solvation model; Fluorene; Alcohol solvents

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INTRODUCTION

Free energy of solvation is an important thermodynamic variable that quantifies the free energy difference between a molecule in the gas phase and the molecule dissolved in a solvent. Free energies of solvation provide valuable information regarding molecular interactions between dissolved solute and surrounding solvent molecules, and can be used to calculate numerical values of partition coefficients that describe the equilibrium distribution of a solute between two immiscible liquid phase. For example, the octanol/water partition coefficient is the free energy of solvation of the solute molecule in wet 1-octanol minus its free energy of solvation in water. Solvation free energies and partition coefficients are of critical importance in many pharmaceutical, environmental and chemical engineering applications. Solute partitioning between two immiscible phases is the basis for all chromatographic separations. Other significant transfer and partitioning processes include the solubility of liquids and solids in water, the solubility of gases in water, blood-brain distribution, general anaesthesia, and the adsorption of organic materials onto clays and soils from aqueous solutions. There are numerous methods available for the estimation of any one of the afore-mentioned transfer processes, but very few methods are based on standard chemical principles that can be applied very generally to all kinds of transfer processes.

One general method is the solvation parameter method of Abraham and coworkers [1–8]. The method is based upon linear free energy relationships for describing the partition of solutes between water and a given solvent

$$\log P = c + rR_2 + s\pi_2^{\mathrm{H}} + a\Sigma\alpha_2^{\mathrm{H}} + b\Sigma\beta_2^{\mathrm{H}} + vV_x \qquad (1)$$

and between the gas phase and a given solvent.

$$\log L = c + rR_2 + s\pi_2^{\mathrm{H}} + a\Sigma\alpha_2^{\mathrm{H}} + b\Sigma\beta_2^{\mathrm{H}} + l\log L^{16} \qquad (2)$$

The dependent variables in Eqs. (1) and (2) are the $\log P$ (the partition coefficient of solute(s) between water and a given solvent) and $\log L$ (Ostwald solubility coefficient). The independent variables are the solute descriptors as follows: R_2 and V_x refer to the excess molar refraction and McGowan volume of the solute, respectively, $\Sigma\alpha_2^H$ and $\Sigma\beta_2^H$ are measures of the solute's hydrogen-bond acidity and hydrogen-bond basicity, π_2^H denotes the solute's dipolarity/polarizability descriptor, and L^{16} is the solute's gas phase dimensionless Ostwald partition coefficient into hexadecane at 298 K. The Ostwald partition coefficient, L, is the inverse of the Henry's law constant (Pa m^3 mol^{-1}). It should be noted that the various *c*, *r*, *s*, *a*, *b*, *v* and *l* coefficients depend on the solvent phase under consideration. The *r*-coefficient gives the tendency of the phase to interact with solutes through polarizability-type interactions, mostly *via* electron pairs. The *s*-coefficient is a measure of the solvent phase dipolarity/polarity, while the *a*- and *b*-coefficients represent the solvent phase hydrogen-bond basicity and hydrogen-bond acidity, respectively. The *l*- and *v*-coefficients are a combination of the work needed to create a solvent cavity wherein the solute will reside, and the general dispersion interaction energy between the solute and solvent phase. In the case of partition coefficients, where two solvent phases are involved, the *c*, *r*, *s*, *a*, *b*, *v* and *l* coefficients represent differences in the solvent phase properties.

Several earlier studies [9–12] developed the computational methodology for determining the various solute descriptors from measured solubility data for crystalline nonelectrolyte solutes dissolved in organic solvents for which the solvent regressional coefficients were known. In the present communication, the process is going to be reversed in that Eqs. (1) and (2) will be used to predict the solubility of fluorene in several dry alcohol solvents. Results of these computations will be compared to experimental solubility data that is measured as part of the present study. To increase our existing solubility data base for polycyclic armotic hydrocarbons, we have measured the solubility of fluorene in 19 different alcohol solvents.

MATERIALS AND METHODS

Fluorene (Aldrich, 98%) was recrystallized several times from methanol. Methanol (Aldrich, 99.8%, anhydrous), ethanol (Aaper Alcohol and Chemical Company, absolute), 1-propanol (Aldrich, 99 + %, anhydrous), 2-propanol (Aldrich, 99+%, anhydrous), 1-butanol (Aldrich, 99.8%, anhydrous), 2-butanol (Aldrich, 99 + %, anhydrous), 2-methyl-l-propanol (Aldrich, 99 + %, anhydrous), 2-methyl-2-propanol (Aldrich, 99.5 + %, anhydrous), 1-pentanol (Aldrich, 99 + %), 3-methyl-1-butanol (Aldrich, 99 + %, anhydrous), 2-pentanol (Acros, 99 + %), 1-hexanol (Alfa Aesar, 99 + %), 1-heptanol (Alfa Aesar, 99 + %), 2-methyl-2-butanol (Acros, 99 + %), 1-octanol (Aldrich, 99 + %, anhydrous), 4-methyl-2-pentanol (Acros, 99 + %), 2-ethyl-1-hexanol (Aldrich, 99 + %), 2-methyl-1-pentanol (Aldrich, 99%) and 1-decanol (Alfa Aesar, 99 + %) were stored over molecular sieves shortly before use to trace water. Gas chromatographic analysis showed solvent purities to be 99.7 mol% or better.

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 for at least 3 days (often longer). Attainment of equilibrium was verified both by repetitive measurements after several additional days and by approaching equilibrium from supersaturation by pre-equilibrating the solutions at a higher temperature. Aliquots of saturated fluorene solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with 2-propanol for spectrophotometric analysis at 280 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 for nine standard solutions. The concentration of fluorene in the standard solutions varied from 8.01×10^{-5} to 2.65×10^{-4} Molar. The calculated molar absorptivity of the standard solutions varied slightly over the concentration range, from $\epsilon \approx 4750\,\mathrm{L\,mol^{-1}\,cm^{-1}}$ (8.01×10^{-5} Molar) to $\epsilon \approx 4550\,\mathrm{L\,mol^{-1}\,cm^{-1}}$ (2.65×10^{-4} Molar).

Experimental molar concentrations were converted to (mass/mass) solubility fractions by multiplying by the molar mass of the solute, volume(s) of volumetric flask(s) used and any dilutions required to place the measured absorbances on the Beer-Lambert law absorbance *versus* concentration working curve, and then dividing by the mass of the saturated solution analyzed. Mole fraction solubilities were computed from (mass/mass) solubility fractions using the molar masses of the solute and solvent. Experimental fluorene solubilities, X_S^{sat}, in the 19 alcohol solvents studied are listed in Table I. Numerical values represent the average of between four and eight independent determinations, with the measurements being reproducible to ± 1.5%.

TABLE I Experimental fluorene mole fraction solubilities, X_S^{sat}, in select organic solvents at 25.0°C

Organic solvent	X_S^{sat}
Methanol	0.00449
Ethanol	0.00743
1-Propanol	0.01232
2-Propanol	0.00949
1-Butanol	0.01686
2-Butanol	0.01206
2-Methyl-1-propanol	0.01006
2-Methyl-2-propanol	0.01016
1-Pentanol	0.02290
2-Pentanol	0.01634
2-Methyl-2-butanol	0.01854
3-Methyl-1-butanol	0.01461
1-Hexanol	0.02757
2-Methyl-1-pentanol	0.01973
4-Methyl-2-pentanol	0.01676
1-Heptanol	0.03503
1-Octanol	0.03884
2-Ethyl-1-hexanol	0.02794
1-Decanol	0.04669

RESULTS AND DISCUSSION

Predictive application of Eqs. (1) and (2) is relatively straightforward if: (a) all solute descriptors and equation coefficients are known, (b) the aqueous solubility of the crystalline solute at 298 K is available, and (c) the saturated vapor pressure of the solid at 298 K has been measured or can be calculated by extrapolating experimental vapor pressure data determined at slightly higher temperatures back to 298 K. These latter two quantities are needed to convert the predicted $\log P$ and $\log L$ values into saturation molar solubilities.

Let the solubility in mol dm^{-1} at 298 K be denoted C_S and C_W, respectively in the organic solvent and in water. The partition coefficient, P, between water and the organic solvent is given by Eq. (3).

$$P = C_S/C_W \quad \text{or} \quad \log P = \log C_S - \log C_W \tag{3}$$

provided that three specific conditions are met. First, the same solid phase must be in equilibrium with the saturation solutions in the organic solvent and in water (i.e., there should be no solvate or hydrate formation). Second, the secondary medium activity coefficient of the solid in the saturated solutions must be unity (or near unity). This condition generally restricts the method to those solutes that are sparingly soluble in water and nonaqueous solvents. Finally, for solutes that are ionized solution, C_W, must refer to the solubility of the neutral form.

If the three fore-mentioned conditions are met, Eqs. (1) and (3) allow one to predict the molar solubility of the solute, C_S, in all organic solvents for which equation coefficients have been determined. Readers are reminded that in selecting equation coefficients, the "dry solvent" values should be used. Equation (1) actually predicts partition coefficients, and for select solvents both "dry" and "wet" equation coefficients have been reported. For solvents that are partially miscible with water, such as 1-butanol and ethyl acetate, partition coefficients calculated using Eq. (3) are not the same as those obtained from direct partition between water (saturated with the organic solvent) and organic solvent (saturated with water). Care must be taken not to confuse the two sets of partitions. In the case of solvents that are fully miscible with water, such as methanol, no confusion is possible. Only one set of equation coefficients have been reported, and the calculated $\log P$ value must refer to the hypothetical partition between the two pure solvents. And for solvents that are "almost" complete immiscible with water, such as alkanes, cyclohexane, dichloromethane, trichloromethane, tetrachloromethane and most aromatic solvents, there should be no confusion because indirect partition through Eq. (3) will be nearly identical to direct partition. Hence, if C_W is known, predicted $\log P$ values based upon Eq. (1) will lead to predicted molar solubilities through Eq. (3). Currently, there are about 40 organic solvents for which "dry" equation coefficients have been determined.

It should be noted that other research groups [13–15] have proposed fairly similar linear solvation energy relationships for estimating partition coefficients of organic solutes between water and an organic solvent. The similar methods employ slightly different solute descriptors, and to our knowledge, all equation coefficients were determined through regressional analysis of direct experimental partition coefficient data. The equations derived from such partition coefficient data are of marginal use in estimating solute solubilities in organic solvents, except in the very special case that the organic solvent is almost completely immiscible with water. Our general solvation method differs from competing methods in that we have tried in recent years, to the extent possible, to build separate data bases for dry and wet solvents. This creates a problem for many of the common organic solvents. There is often very little experimental data available, and the tendency is to combine available organic solvent/water partition coefficient measurements (wet solvent) with saturation solubilities, binary liquid-vapor equilibria data, and infinite dilution activity coefficients determined from measured gas chromatographic solute retention volumes on the organic solvent stationary phase [16,17]. Lack of experimental data is the reason that we have been able to deduce *c*, *r*, *s*, *a*, *b*, *v* and *l* coefficients for only 40 or so dry solvents. Equations coefficients are tabulated in Table II for methanol,

TABLE II Coefficients in Eqs. (1) and (2) for various processes[a]

Process/solvent	*c*	*r*	*s*	*a*	*b*	*v/l*[b]
A. Water to solvent: Eq. (1)						
Methanol (dry)	0.329	0.299	−0.671	0.080	−3.389	3.512
Ethanol (dry)	0.208	0.409	−0.959	0.186	−3.645	3.928
1-Propanol (dry)	0.147	0.494	−1.195	0.495	−3.907	4.048
2-Propanol (dry)	0.063	0.320	−1.024	0.445	−3.824	4.067
1-Butanol (dry)	0.152	0.437	−1.175	0.098	−3.914	4.119
1-Pentanol (dry)	0.080	0.521	−1.294	0.208	−3.908	4.208
1-Hexanol (dry)	0.044	0.470	−1.153	0.083	−4.057	4.249
1-Heptanol (dry)	−0.026	0.491	−1.258	0.035	−4.155	4.415
1-Octanol (dry)	−0.034	0.490	−1.048	−0.028	−4.229	4.219
1-Decanol (dry)	−0.062	0.754	−1.461	0.063	−4.053	4.293
(Gas to water)	−0.994	0.577	2.549	3.813	4.841	−0.869
B. Gas to solvent: Eq. (2)						
Methanol (dry)	−0.004	−0.215	1.173	3.701	1.432	0.769
Ethanol (dry)	0.012	−0.206	0.789	3.635	1.311	0.853
1-Propanol (dry)	−0.028	−0.185	0.648	4.022	1.043	0.869
2-Propanol (dry)	−0.060	−0.335	0.702	4.017	1.040	0.893
1-Butanol (dry)	−0.039	−0.276	0.539	3.781	0.995	0.934
1-Pentanol (dry)	−0.042	−0.277	0.526	3.779	0.983	0.932
1-Hexanol (dry)	−0.035	−0.298	0.626	3.726	0.729	0.936
1-Heptanol (dry)	−0.062	−0.168	0.429	3.541	1.181	0.927
1-Octanol (dry)	−0.119	−0.203	0.560	3.576	0.702	0.940
1-Decanol (dry)	−0.136	−0.038	0.325	3.674	0.767	0.947
(Gas to water)	−1.271	0.822	2.743	3.904	4.814	−0.213

[a] The solvents denoted as "dry" are those for which partitions refer to transfer to the pure dry solvent. The other partitions are from water (more correctly water saturated with solvent) to the solvent saturated with water (see text); Coefficient of V_x in processes *A* and coefficient of Log L^{16} in processes *B*.

ethanol, 1-propanol, 2-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol and 1-decanol. These are the only alcohols for which equation coefficients have been determined. The actual numerical values may differ slightly from values reported in earlier publications. Coefficients are periodically revised when additional experimental data becomes available.

Saturation solubilities can also be calculated from predicted log L values based upon Eq. (2), provided that the solid saturated vapor pressure at 298 K, VP°, is available. VP° can be transformed into the gas phase concentration, C_G and the gas–water and gas–solvent partitions, L_W and L_S, can be obtained through

$$L_W = C_W/C_G \quad \text{or} \quad \log L_W = \log C_W - \log C_G \tag{4}$$

$$L_S = C_S/C_G \quad \text{or} \quad \log L_S = \log C_S - \log C_G \tag{5}$$

Eqs. (4) and (5), respectively. As before, the predictive method will be valid if conditions discussed above are met. In the case of the published log L correlations most of the equation coefficients pertain to either "dry" solvents or solvents that are "almost" completely immiscible with water.

Table III compares the observed fluorene molar solubilities, C_S^{exp}, to values calculated using the Abraham general solvation model The model predicts $\log P$ and $\log L$ partitions, which were then converted to molar solubilities through Eqs. (3) and (4) using Log $C_W = -5.00$ [18] and Log $C_G = -7.45$ [19,20]. Solute descriptors used in the predictions were: $R_2 = 1.588$; $\pi_2^H = 1.06$; $\Sigma\alpha_2^H = 0.00$; $\Sigma\beta_2^H = 0.25$; $V_x = 1.3565$ and $\log L^{16} = 6.922$. For comparison purposes, all measured mole fraction solubility data, X_S^{exp}, were converted to molarities by dividing X_S^{exp} by the ideal molar volume of the saturated solution (i.e., $C_S^{sat} \approx X_S^{exp}/[X_S^{exp} V_{solute} + (1 - X_S^{exp}) V_{solvent}]$). The molar volume of the hypothetical subcooled liquid fluorene, $V_{solute} = 147.0\,\text{cm}^3\,\text{mol}^{-1}$ was estimated based upon the group contribution method of Shahidi *et al.* [21]. Solvent molar volumes used in these conversions are given elsewhere [22–25]. Any errors resulting from our estimation of the fluorene's hypothetical subcooled liquid molar volume, V_{solute}, or the ideal molar volume approximation should have negligible effect on the calculated C_S^{exp} values. Fluorene is fairly insoluble in many

TABLE III Comparison between experimental fluorene molar solubilities, C_S^{exp}, and predicted values based upon the Abraham general solvation model (Eqs. (1) and (2))

Solvent	C_S^{exp}	*Eq.* (1)		*Eq.* (2)	
		C_S^{pred}	*% Dev.*[a]	C_S^{pred}	*% Dev.*[a]
Methanol (dry)	0.1090	0.1021	− 6.3	0.1345	23.4
Ethanol (dry)	0.1252	0.1811	44.6	0.2009	60.4
1-Propanol (dry)	0.1621	0.1507	− 7.0	0.1552	− 4.3
2-Propanol (dry)	0.1223	0.1114	− 8.9	0.1390	13.6
1-Butanol (dry)	0.1814	0.1629	− 10.2	0.2296	26.6
1-Pentanol (dry)	0.2092	0.1849	− 11.6	0.2104	0.6
1-Hexanol (dry)	0.2192	0.2080	− 5.1	0.2291	4.5
1-Heptanol (dry)	0.2465	0.2344	− 4.9	0.2443	− 0.9
1-Octanol (dry)	0.2460	0.1991	− 19.1	0.2376	− 3.4
1-Decanol (dry)	0.2464	0.2494	1.2	0.2786	13.1
Average Absolute Deviation			11.9		15.1

[a] % Dev = 100 $(C_S^{pred} - C_S^{exp})/C_S^{exp}$.

of the solvents considered, and the $X_S^{exp}\ V_{solute}$ term contributes very little to the molar volume of the saturated solution.

Examination of the numerical entries in Table III reveals that Eqs. (1) and (2) provide a very reasonable (though by no means perfect) estimation of the solubility behavior of fluorene in the 10 alcohol solvents for which equation coefficients are available. Overall average absolute deviations between predicted and observed values were 11.9 and 15.1% for Eqs. (1) and (2), respectively. Expressed on a logarithmic molar scale basis, the Abraham general solvation model estimates the solubilities to within ± 0.05 and ± 0.06 log units, which is less than the standard deviations associated with the *c*, *r*, *s*, *a*, *b*, *v* and *l* coefficients for the individual solvent systems. Standard deviations for most of the individual solvent correlations fell in the range of ± 0.12–± 0.20 log units. Our past experience in using different solution models has been than the better solution models will generally give predicted values that fall within ± 40% or so of the observed solute solubilities. The Abraham general solvation model meets this criterion. Fluorene solubility data that could not be predicted because of lack of equation coefficients will be used in subsequent studies to generate correlation equations for additional alcohol solvents. Finally, it should be noted that the present method is not limited to the prediction of fluorene solubilities in alcohols. We discuss these particular predictions, because we have measured the solubilities in alcohols, but the method can be used to predict solubilities in other solvents, and to predict various biological and environmental properties [5,6,8,26].

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