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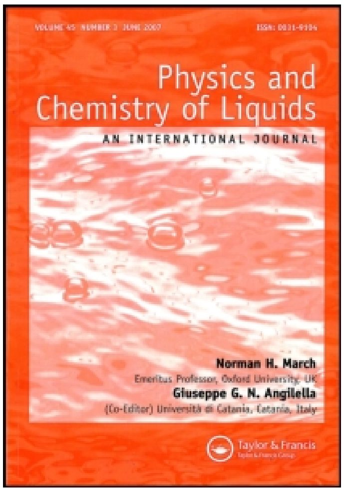

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Solubility of 9-Fluorenone in Organic Nonelectrolyte Solvents: Comparison of Observed Versus Predicted Values Based Upon Mobile Order Theory

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SOLUBILITY OF 9-FLUORENONE IN ORGANIC NONELECTROLYTE SOLVENTS: COMPARISON OF OBSERVED *VERSUS* PREDICTED VALUES BASED UPON MOBILE ORDER THEORY

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Experimental solubilities are reported at 25.0°C for 9-fluorenone dissolved in 40 different organic nonelectrolyte solvents containing ether-, chloro-, hydroxy-, cyano and *t*-butyl-functional groups. Results of these measurements are used to test the applications and limitations of expressions derived from Mobile Order theory. For the 29 solvents for which predictions could be made, computations show that Mobile Order theory does provide fairly reasonable estimates of the saturation mole fraction solubilities. Average absolute deviation between predicted and observed values is 39.3%.

Keywords: 9-Fluorenone solubilities; Organic nonelectrolyte solvents; Solubility predictions

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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 phases. 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. Correlations have been derived for predicting brain–blood partitioning of organic solutes from solutes' measured

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and/or calculated free energies of solvation [1,2], and for estimating aqueous solubilities, soil adsorptions, bioaccumulations and toxicities of organic compound from experimental octanol–water partition coefficient data [3–11].

Historically, many of the very early studies focussed exclusively on developing correlational equations based upon octanol–water partition coefficients. Recent studies have shown that the octanol–water partition coefficient may not necessarily be the best indicator of how likely it is for a particular solute molecule to penetrate a lipid bilayer, skin, brain or central nervous system, or to accumulate in different tissues and body organs. Experimental studies have been expanded to include additional organic solvents, as well as aqueous micellar solvent media, and to use solute descriptors calculable from structural considerations and/or easily measured thermodynamic quantities.

In this regard, Abraham and coworkers [12–19] developed expressions for describing the partition of solutes between water and a given solvent

$$\log P = c + r \cdot R_2 + s \cdot \pi_2^H + a \cdot \sum \alpha_2^H + b \cdot \sum \beta_2^H + v \cdot V_x \tag{1}$$

and between the gas phase and a given solvent

$$\log L = c + r \cdot R_2 + s \cdot \pi_2^H + a \cdot \sum \alpha_2^H + b \cdot \sum \beta_2^H + l \cdot \mathrm{Log}\, L^{16} \tag{2}$$

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, $\sum \alpha_2^H$ and $\sum \beta_2^H$ are measures of the solute's hydrogen-bond acidity and hydrogen-bond basicity, π_2^H denotes the solute's dipolarity/polarizability descriptor, and Log 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 $mole^{-1}$). 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 [20–24] 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. Solutes studies included *trans*-stilbene, diuron, monuron, buckminsterfullerene, benzil and ferrocene. Diuron and monuron had the larger numerical values of the $\sum \alpha_2^H$ and $\sum \beta_2^H$ solute descriptors. Continued development of additional correlation equations requires the establishment of large solubility and activity coefficient databases for each solvent system to be studied. The databases

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should contain solutes that span as wide of a range of solute descriptors as possible. For this reason, we are in the process of measuring solubility data for several crystalline organic compounds. In the present communication we report 9-fluorenone solubilities at 25°C in 40 different organic solvents of varying polarity and hydrogen bonding capability. Results of these measurements are used to further test the applications and limitations of predictive expressions derived from Mobile Order theory. Subsequent papers will consider the mathematical correlation of 9-fluorenone solubilities based upon other solution models.

MATERIALS AND METHODS

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9-Fluorenone (Aldrich, 98%) was recrystallized several times from anhydrous methanol before use. *n*-Hexane (Aldrich, 99%), *n*-heptane (Aldrich, HPLC), *n*-octane (Aldrich 99+ %, anhydrous), *n*-nonane (TCI, 99+%), *n*-decane (TCI, 99+%), *n*-hexadecane (Aldrich, 99%), cyclohexane (Aldrich, HPLC), methylcyclohexane (Aldrich, 99+%, anhydrous), cyclooctane (Lancaster Synthesis, 99+%), 2,2,4-trimethylpentane (Aldrich, HPLC), benzene (Aldrich, HPLC, 99.9+%), toluene (Aldrich, 99.8%, anhydrous), methanol (Aldrich, 99.9+%), ethanol (Aaper Alcohol and Chemical Company, absolute), 1-propanol (Aldrich, 99+%, anhydrous), 2-propanol (Aldrich, 99+%, anhydrous), 1-butanol (Aldrich HPLC, 99.8+%), 2-butanol (Aldrich, 99+%, anhydrous), 1-pentanol (Aldrich, 99+%), 1-hexanol (Alfa Aesar, 99+%), 1-heptanol (Alfa Aesar, 99+%), 1-octanol (Aldrich, 99+%, anhydrous), 1-decanol (Alfa Aesar, 99+%), 2-pentanol (Acros 99+%), 2-methyl-2-butanol (Acros, 99+%), 2-methyl-1-propanol (Aldrich, 99+%, anhydrous), 3-methyl-1-butanol (Aldrich, 99+%, anhydrous), 4-methyl-2-pentanol (Acros, 99+%), 2-ethyl-1-hexanol (Aldrich, 99+%), 2-methyl-1-pentanol (Aldrich, 99%), 2-methyl-2-propanol (Arco Chemical Company, 99+%), cyclopentanol (Aldrich, 99%), dibutyl ether (Aldrich, 99%), methyl *tert*-butyl ether (Arco, 99.9+%), diisopropyl ether (Aldrich, 99%, anhydrous), carbon tetrachloride (Aldrich, 99.5+%, anhydrous), dichloromethane (Aldrich, 99.8%, anhydrous), acetonitrile (Aldrich, 99.8%, anhydrous), propionitrile (Aldrich, 99%) and butyronitrile (Aldrich, 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.

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 three days (often longer). Attainment of equilibrium was verified both by repetitive measurements after several additional days and by approaching equilibrium from supersaturation by preequilibrating the solutions at a higher temperature. Aliquots of saturated 9-fluorenone 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 393 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 calculated molar absorptivity of 9-fluorenone at 393 nm varied slightly with concentration, ranging from a value of $\varepsilon \approx 241.5\,\mathrm{L\,mol^{-1}\,cm^{-1}}$ (1.62×10^{-3} M) to $\varepsilon \approx 239.0\,\mathrm{L\,mol^{-1}\,cm^{-1}}$ (5.40×10^{-3} M).

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Experimental molar concentrations were converted to (mass/mass) solubility fractions by multiplying by the molar mass of 9-fluorenone, 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 mole fraction solubilities, X_A^{sat}, are listed in Table I for 9-fluorenone dissolved in 40 organic solvents. Numerical values represent the average of between four and eight independent determinations, with the measurements were reproducible to within ± 1.5%.

TABLE I Comparison between experimental 9-fluorenone mole fraction solubilities and predicted values based upon mobile order theory

Organic Solvent	$(X_A^{sat})^{exp,a}$	$(X_A^{sat})^{calc}$	% *Dev*[b]
n-Hexane	0.01285	0.01390	8.2
n-Heptane	0.01565	0.01502	−4.0
n-Octane	0.01819	0.01770	−2.7
n-Nonane	0.02073	0.02140	3.2
n-Decane	0.02316	0.02275	−1.8
n-Hexadecane	0.03445	0.03488	1.2
Cyclohexane	0.01643	0.01855	12.9
Methylcyclohexane	0.01778	0.02084	17.2
Cyclooctane	0.02420	0.02919	20.6
2,2,4-Trimethylpentane	0.01136	0.01071	−5.7
Benzene	0.2725	0.2526	−7.3
Toluene	0.2514	0.1880	−25.2
Dibutyl ether	0.06159	0.1187	92.7
Diisopropyl ether	0.05024		
Methyl *tert*-butyl ether	0.09097		
Dichloromethane	0.3964	0.3155	−20.4
Carbon tetrachloride	0.1844	0.1197	−35.1
Acetonitrile	0.1007	0.3088	206.6
Propionitrile	0.1663		
Butyronitrile	0.1907		
Methanol	0.01623	0.01235	−23.9
Ethanol	0.02471	0.01435	−41.9
1-Propanol	0.02954	0.01614	−45.4
2-Propanol	0.02241	0.01993	−11.1
1-Butanol	0.03516	0.01984	−43.6
2-Butanol	0.03138	0.01392	−55.6
2-Methyl-1-propanol	0.02385	0.01023	−57.1
2-Methyl-2-propanol	0.02913	0.00801	−72.5
1-Pentanol	0.04495	0.02009	−55.3
2-Pentanol	0.03813		
3-Methyl-1-butanol	0.03391		
2-Methyl-2-butanol	0.04422		
1-Hexanol	0.05114	0.01748	−65.8
2-Methyl-1-pentanol	0.04497		
4-Methyl-2-pentanol	0.03635		
1-Heptanol	0.06094	0.01976	−67.6
1-Octanol	0.06761	0.02181	−67.7
2-Ethyl-1-hexanol	0.05484		
1-Decanol	0.07858	0.02533	−67.8
Cyclopentanol	0.07347		

[a]Numerical values represent the average of between four and eight independent determinations, with the measurements being reproducible to ±1.5%; [b]Deviations (%) = $100[(X_A^{sat})^{calc} - (X_A^{sat})^{exp}]/(X_A^{sat})^{exp}$.

RESULTS AND DISCUSSION

Solvents listed in Table I include both noncomplexing alkanes and self-associating alcohols. Of the many solutions models proposed in recent years, mobile order theory is perhaps the only one that is capable of describing solute behavior in such a wide range of solvent mixtures. The basic model [25–32] assumes that all molecular groups perpetually move, and that neighbors of a given kind of external atom in a molecule constantly change identity. All molecules of a given kind dispose of the same volume, equal to the total volume V of the liquid divided by the number N_A of molecules of the same kind, i.e., $\text{Dom}\, A = V/N_A$. The center of this domain perpetually moves. The highest mobile disorder is achieved whenever groups visit all parts of their domain without preference. Preferential contacts lead to deviations with respect to this "random" visiting. This is especially true in the case of hydrogen-bonding as specific interactions result in a specific orientation of the "donor" molecule with respect to an adjacent "acceptor" molecule.

In the case of an inert crystalline solute dissolved in a self-associating solvent, mobile order theory expresses the volume fraction saturation solubility, ϕ_A^{sat}, as

$$\begin{aligned}\ln \phi_A^{\text{sat}} &= \ln a_A^{\text{solid}} - 0.5(1 - V_A/V_{\text{solvent}})\phi_{\text{solvent}} \\ &\quad + 0.5 \ln[\phi_A^{\text{sat}} + \phi_{\text{solvent}}(V_A/V_{\text{solvent}})] - \phi_{\text{solvent}}^2 V_A(\delta'_A - \delta'_{\text{solvent}})^2 (RT)^{-1} \\ &\quad - r_{\text{solvent}}(V_A/V_{\text{solvent}})\phi_{\text{solvent}} \end{aligned} \tag{3}$$

where the r_{solvent} (V_A/V_{solvent}) ϕ_{solvent} term represents the contributions resulting from hydrogen-bond formation between the solvent molecules. For most of the published applications, r_{solvent} was assumed to be unity for strongly associated solvents with single hydrogen-bonded chains such as monofunctional alcohols, to be two for water or diols, and to equal zero for nonassociated solvents such as saturated hydrocarbons. A more exact value for alcoholic solvents can be calculated based upon

$$r_{\text{solvent}} = (K_{\text{solvent}}\phi_{\text{solvent}}/V_{\text{solvent}})/(1 + K_{\text{solvent}}\phi_{\text{solvent}}/V_{\text{solvent}}) \tag{4}$$

with a numerical value of $K_{\text{solvent}} = 5000\,\text{cm}^3\,\text{mol}^{-1}$ assumed for all monofunctional alcohols.

If complexation does occur between the crystalline solute and solvent

$$\begin{aligned}\ln \phi_A^{\text{sat}} &= \ln a_A^{\text{solid}} - 0.5(1 - V_A/V_{\text{solvent}})\phi_{\text{solvent}} \\ &\quad + 0.5 \ln[\phi_A^{\text{sat}} + \phi_{\text{solvent}}(V_A/V_{\text{solvent}})] - \phi_{\text{solvent}}^2 V_A(\delta'_A - \delta'_{\text{solvent}})^2 (RT)^{-1} \\ &\quad + \ln[1 + \phi_{\text{solvent}}(K_{A\text{Solvent}}/V_{\text{solvent}})] \end{aligned} \tag{5}$$

then an additional term involving the solute–solvent equilibrium constant, $K_{A\text{Solvent}}$, must be introduced to describe the solubility enhancement that arises as a result of specific interactions. A slightly more complex expression applies in the case of solute complexation with a self-associating solvent. The expression's mathematical form depends to a large extent upon the number and type of hydrogen-bond acid and hydrogen-bond base functional groups in the solute molecule being studied.

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The symbols δ'_A and δ'_{solvent} denote the modified solubility parameters of the solute and solvent, respectively, V_i is the molar volume, and a_A^{solid} is the activity of the solid solute. This latter quantity is defined as the ratio of the fugacity of the solid to the fugacity of the pure hypothetical supercooled liquid. The numerical value of a_A^{solid} can be computed from

$$\ln a_A^{\text{solid}} = -\Delta H_A^{\text{fus}}(T_{\text{mp}} - T)/(RT\,T_{\text{mp}}) + (\Delta C_{p,A}/RT)(T_{\text{mp}} - T) - (\Delta C_{p,A}/T)\ln(T_{\text{mp}}/T) \tag{6}$$

the solute's molar enthalpy of fusion, ΔH_A^{fus}, and heat capacity difference, $\Delta C_{p,A}$, at the normal melting point temperature, T_{mp}. Contributions from nonspecific interaction are incorporated into mobile order theory through the $\phi_{\text{solvent}}^2 V_A(\delta'_A - \delta'_{\text{solvent}})^2(RT)^{-1}$ term.

It is noted that other research groups have treated nonspecific interactions differently, and have assumed solution models other than the Scatchard–Hildebrand solubility parameter theory. For example, Ruelle [33] in predicting solubilities in systems involving hydrogen-bond formation between a dissolved solute and surrounding solvent molecules, modified the Scatchard–Hildebrand expression by multiplying it by the fraction of time during which the solute is not bound to the solvent [i.e., during which the distribution between the solvent and unbound solute molecules can still be considered to occur at random]. Ruelle's treatment further assumed that nonspecific interactions involving the bound solute were negligible. The theoretical justification for Ruelle's modification was not given, and it is not clear to us what mathematical form the integral $(\Delta G_{A\text{Solvent}})_{\text{phys}}$ for the binary solution would have to take in order to give

$$(\Delta G_A)_{\text{phys}} = \{1/[1.0 + \max(K_{\text{Oi}}, K_{\text{OHi}})(\phi_{\text{solvent}}/V_{\text{solvent}})]\} \cdot \phi_{\text{solvent}}^2 V_A(\delta'_A - \delta'_{\text{solvent}})^2 \tag{7}$$

whenever $(\Delta G_{A\text{Solvent}})_{\text{phys}}$ is differentiated with respect to the number of moles of solute present. The differentiation is required in deriving the solubility equation. Readers are reminded that any modification to the $(\Delta G_A)_{\text{phys}}$ expression must also show up in the corresponding $(\Delta G_{\text{Solvent}})_{\text{phys}}$ expression, the latter expression being obtained by differentiating $(\Delta G_{A\text{Solvent}})_{\text{phys}}$ with respect to the number of molecules of solvent. In Eq. (7) $\max(K_{\text{Oi}}, K_{\text{OHi}})$ stands for the association constant governing the strongest intermolecular H-bond displayed by the molecular groups in solution. We have elected to use the Scatchard–Hildebrand solubility parameter theory, rather than the Ruelle modification, because we have serious reservations about whether nonspecific interactions for bound molecules are truly negligible as assumed by Ruelle in proposing Eq. (7).

Predictive application of Eqs. (3) and (5) is relatively straightforward. First, an average numerical value of $\delta'_{\text{flrnone}} = 21.91\,\text{MPa}^{1/2}$ is computed by requiring that each equation (with $r_{\text{solvent}} = 0$ and/or $K_{A\text{Solvent}} = 0$) perfectly describes 9-fluorenone mole fraction solubility data in *n*-hexane ($\delta'_{\text{flrnone}} = 21.99\,\text{MPa}^{1/2}$), *n*-heptane ($\delta'_{\text{flrnone}} = 21.86)\,\text{MPa}^{1/2}$, and *n*-octane ($\delta'_{\text{flrnone}} = 21.88\,\text{MPa}^{1/2}$). The numerical value of $a_A^{\text{solid}} = 0.3028$ is calculated using Eq. (6) with $\Delta H_A^{\text{fus}} = 18.12\,\text{kJ mol}^{-1}$ and $T_{\text{mp}} = 356.4\,\text{K}$ [34]. The two heat capacity terms in Eq. (6) were set equal to zero as we were unable to find heat capacity data for the subcooled liquid solute. A numerical

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value of $V_{\text{flrnone}} = 146.0\,\text{cm}^3\,\text{mol}^{-1}$ was used for the molar volume of the hypothetical subcooled liquid solute.

Table I summarizes the predictive ability of Mobile Order theory for the various organic solvents for which both 9-fluorenone solubility data and modified solubility parameters could be found. Solvent molar volumes and modified solubility parameters are listed in Table II. We were unable to find modified solubility parameters for all of the secondary and branched alcohols. The modified solubility parameters account for only nonspecific interactions, and in the case of the alcoholic solvents the hydrogen-bonding contributions have been removed. Numerical values of δ'_{solvent} were obtained from published compilations [28,29,31,32], and were either deduced by regressing actual solubility data of solid *n*-alkanes in organic solvents in accordance with the configurational entropic model of Huyskens and Haulait–Pirson [35] or estimated using known values for similar organic solvents. Examination of the entries in Table I reveals that Mobile Order theory does provide fairly reasonable (though by no means perfect) estimates of the solubility behavior of 9-fluorenone in a wide range of organic solvents. Average absolute deviation between predicted and observed values is 39.3%.

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TABLE II Solvent and solute properties used in mobile order predictions

Component (i)	V_i (cm^3 mol^{-1})	δ'_i (MPa$^{1/2}$)[a]
n-Hexane	131.51	14.56
n-Heptane	147.48	14.66
n-Octane	163.46	14.85
n-Nonane	179.87	15.07
n-Decane	195.88	15.14
n-Hexadecane	294.12	15.61
Cyclohexane	108.76	14.82
Methylcyclohexane	128.32	15.00
Cyclooctane	134.9	15.40
2,2,4-Trimethylpentane	166.09	14.30
Benzene	89.4	18.95
Toluene	106.84	18.10
Dibutyl ether	170.3	17.45
Methanol	40.7	19.25
Ethanol	58.7	17.81
1-Propanol	75.10	17.29
2-Propanol	76.90	17.60
1-Butanol	92.00	17.16
2-Butanol	92.4	16.60
2-Methyl-1-propanol	92.8	16.14
2-Methyl-2-propanol	94.3	15.78
1-Pentanol	108.6	16.85
1-Hexanol	125.2	16.40
1-Heptanol	141.9	16.39
1-Octanol	158.3	16.38
1-Decanol	191.6	16.35
Tetrachloromethane	97.08	17.04
Dichloromethane	64.5	20.53
Acetonitrile	52.9	23.62
9-Fluorenone[b]	146.0	21.91[c]

[a]Tabulated values are taken from a compilation given in Ruelle *et al.* [28,29,31,32]; [b]The numerical value of $a_A^{\text{solid}} = 0.3028$ was calculated from Eq. (8) using $\Delta H_A^{\text{fus}} = 18.12\,\text{kJ}\,\text{mol}^{-1}$ and $T_{\text{mp}} = 356.4\,\text{K}$ [34]; [c]Numerical value was calculated using the measured 9-fluorenone mole fraction solubilities in *n*-hexane, *n*-heptane and *n*-octane, in accordance with Eqs. (3) and (5); with $r_{\text{solvent}} = 0$ and/or $K_{A\text{Solvent}} = 0$.

Readers are reminded that in evaluating the applicability of Mobile Order theory one must realize that many of these particular systems are highly nonideal, and that the experimental solubility data covers over a 39-fold range in mole fraction. Had an ideal solution been assumed, then the predicted mole fraction solubility would be $X_A^{\text{sat}} = a_A^{\text{solid}} = 0.3028$ for each solvent. The ideal solution approximation corresponds to a considerably larger average absolute deviation of 958.0% between predicted and observed values for the nonalcoholic solvents studied.

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