

Solubility of Anthracene and Phenanthrene in Ethanol + 2,2,4-Trimethylpentane Mixtures at Different Temperatures

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ABSTRACT: Solubility of anthracene and phenanthrene in binary mixtures of ethanol + 2,2,4-trimethylpentane at (298.2, 308.2, and 318.2) K are reported. Five numerical methods were used to predict the solubility of anthracene and phenanthrene in the studied binary solvent mixtures, and the mean relative deviation (MRD) was used as an error criterion. The MRD values for studied solvents are in acceptable range.

INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) are among environmental pollutants with very low aqueous solubility values. Anthracene (with aqueous solubility of $0.0076 \text{ mg}\cdot\text{L}^{-1}$) and phenanthrene (with aqueous solubility of $1.20 \text{ mg}\cdot\text{L}^{-1}$) are among the most commonly found PAHs in the environment.¹ Anthracene and phenanthrene are two isomeric forms of the simplest tricyclic aromatic hydrocarbon (Figure 1) and were used as model compounds in this work. Phenanthrene has lower molecular total energy, and it is more stable than anthracene according to *ab initio* studies using molecular orbital method in the gas phase.²

Solubility alteration of chemicals is required in many industrial applications, and the solvent mixing or cosolvency is one of the most frequent and feasible methods used in the industry. Using different ratios of the solvents, a wide range of solubility for a given compound can be achieved. The next parameter which could be employed in the chemical industry is the changing temperature of the system which make a significant contribution in solubilization or crystallization of a compound. Finding an optimum solvent composition and the appropriate temperature in solubility investigations is usually obtained by trial and error which is both time-consuming and costly.

SOLUBILITY MODELS

Numerous predictive models have been introduced to replace the trial-and-error approach or at least reduce the number of required experimental data.¹ One of these models, is the Jouyban–Acree model which correlates the solubility of a solute in binary solvent mixtures at various temperatures.³

$$\ln X_{m,T}^{\text{Sat}} = x_1 \cdot \ln X_{1,T}^{\text{Sat}} + x_2 \cdot \ln X_{2,T}^{\text{Sat}} + \frac{x_1 \cdot x_2}{T} \cdot \sum_{i=0}^2 J_i (x_1 - x_2)^i \quad (1)$$

where $X_{m,T}^{\text{Sat}}$ is the solute mole fraction solubility in the mixed solvents at temperature T ; x_1 and x_2 are the mole fractions of

solvents 1 and 2 in the absence of the solute; $X_{1,T}^{\text{Sat}}$ and $X_{2,T}^{\text{Sat}}$ denote the mole fraction solubility of the solute in monosolvents 1 and 2; and J_i terms are the solvent–solvent and solute–solvent interaction coefficients. Our previous results showed that the model could be trained using the experimental data at 298.2 K and be used to predict the solubility at other temperatures of interest with acceptable error.⁴ These coefficients could also be computed using a minimum number of experimental solubility data in binary solvents and then be employed to predict solubility at other solvent compositions. To provide trained versions of the model to predict the solubility in binary solvents without employing solubility data in mixed solvents, a number of attempts were made. The binary interaction terms (J terms) have been correlated with the Hildebrand solubility parameters of the solvents and solutes. The reported quantitative structure property relationships (QSPR) using the Hildebrand solubility parameters are:⁵

$$J_0 = 0.039(\delta_1 - \delta_s) + 0.154(\delta_2 - \delta_s) + 0.078(\delta_1 - \delta_s)^2 - 0.063(\delta_2 - \delta_s)^2 \quad (2)$$

$$J_1 = 0.059(\delta_1 - \delta_s) + 0.023(\delta_2 - \delta_s) + 0.036(\delta_1 - \delta_s)^2 - 0.025(\delta_2 - \delta_s)^2 \quad (3)$$

$$J_2 = 0.023(\delta_1 - \delta_s) - 0.006(\delta_2 - \delta_s) + 0.012(\delta_1 - \delta_s)^2 - 0.015(\delta_2 - \delta_s)^2 \quad (4)$$

where δ_1 , δ_2 , and δ_s represent the solubility parameter (expressed as $(\text{MPa}^{1/2})$) of solvent 1, solvent 2, and the solute, respectively. The numerical values for the solubility parameters of anthracene, phenanthrene, ethanol, and 2,2,4-trimethylpentane are 19.5, 19.9, 26.6, and 14.0, respectively.

In another attempt, the J terms have been described using Abraham solvent and solute parameters.⁶ It is shown that these

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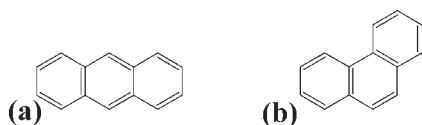


Figure 1. Structures of (a) anthracene and (b) phenanthrene.

models can be applied to obtain calculated solubility data in binary solvent mixtures with acceptable errors.^{6–9} The J_i coefficients are described as

$$J_0 = 0.028 + 2.123(c_1 - c_2)^2 - 0.160E(e_1 - e_2)^2 + 0.282S(s_1 - s_2)^2 + 1.713B(b_1 - b_2)^2 + 2.006V(v_1 - v_2)^2 \quad (5)$$

$$J_1 = 0.033 + 0.670(c_1 - c_2)^2 - 0.477E(e_1 - e_2)^2 + 0.051S(s_1 - s_2)^2 + 0.476B(b_1 - b_2)^2 + 0.234V(v_1 - v_2)^2 \quad (6)$$

$$J_2 = 0.022 + 2.024(c_1 - c_2)^2 - 0.204E(e_1 - e_2)^2 + 0.034S(s_1 - s_2)^2 + 0.243B(b_1 - b_2)^2 + 0.848V(v_1 - v_2)^2 \quad (7)$$

for water-to-solvent Abraham solvent parameters, and

$$J_0 = 0.062 + 0.118(c_1 - c_2)^2 - 0.332E(e_1 - e_2)^2 + 0.410S(s_1 - s_2)^2 + 2.399B(b_1 - b_2)^2 + 15.715L(l_1 - l_2)^2 \quad (8)$$

$$J_1 = 0.103 + 1.864(c_1 - c_2)^2 - 1.590E(e_1 - e_2)^2 + 0.119S(s_1 - s_2)^2 + 1.010B(b_1 - b_2)^2 - 9.493L(l_1 - l_2)^2 \quad (9)$$

$$J_2 = 0.008 + 1.075(c_1 - c_2)^2 - 0.053E(e_1 - e_2)^2 + 0.084S(s_1 - s_2)^2 + 0.414B(b_1 - b_2)^2 + 7.727L(l_1 - l_2)^2 \quad (10)$$

for gas-to-solvent Abraham solvent parameters. In these equations, c , e , s , b , v , and l are the Abraham solvent coefficients¹⁰ (Table 1); E is the excess molar refraction, S is the dipolarity/polarizability, B is the hydrogen bond basicity, V is one percent of McGowan volume, and L is the logarithm of gas-hexadecane partition coefficient of the solute at 298.15 K.¹⁰

The solubilities of anthracene and phenanthrene in binary solvent mixtures have been extensively studied.^{7–9,11,12} To the best of our knowledge, there is no reported solubility data for anthracene and phenanthrene in ethanol + 2,2,4-trimethylpentane mixtures in the literature. The aims of this study are: (1) The solubilities of anthracene and phenanthrene in ethanol + 2,2,4-trimethylpentane at (298.2, 308.2, and 318.2) K are reported. (2) The constants of the Jouyban–Acree model for anthracene and phenanthrene in ethanol + 2,2,4-trimethylpentane mixtures are calculated. (3) The possibility of predicting the solubility of solutes at other temperatures using the trained model at 298.2 K is shown. (4) The Jouyban–Acree model combined with the Hildebrand solubility parameters is applied to predict the solubility of anthracene and phenanthrene in the binary solvent

Table 1. The Abraham Solvent Coefficients of Water and 2,2,4-Trimethylpentane¹⁰

water-to-solvent	c	e	s	a	b	v
ethanol	0.208	0.409	−0.959	0.186	−3.645	3.928
2,2,4-trimethylpentane	0.288	0.382	−1.668	−3.639	−5.000	4.461
gas-to-solvent	c	e	s	a	b	l
ethanol	0.012	−0.206	0.789	3.635	1.311	0.853
2,2,4-trimethylpentane	0.275	−0.244	0.000	0.000	0.000	0.972

mixtures at various temperatures. (5) The Jouyban–Acree model combined with Abraham parameters is applied to predict the solubility of solutes in the binary solvent mixtures at various temperatures. (6) The applicability of a new approach to predict the density of saturated solutions using the density of solute free solvent mixtures is also evaluated.^{13,14}

EXPERIMENTAL METHOD

Materials. Anthracene (purity 0.96 in mass fraction) was purchased from Fluka, and it was recrystallized several times using 2-propanone and ethyl acetate to yield a purified sample having a melting point of 488 K. Its purity was checked by a thin layer chromatography method,¹⁵ and also the measured solubilities in ethanol and 2,2,4-trimethylpentane were compared with the corresponding data from the literature. Phenanthrene (purity > 0.98 in mass fraction) was purchased from Merck. It was recrystallized for several times using 2-propanone. A thin layer chromatography method¹⁵ and melting temperature determination equal to 372.15 K revealed its purity. Also, solubilities in ethanol and 2,2,4-trimethylpentane are in good agreement with previously published data.^{8,10,16–18} 2,2,4-Trimethylpentane (> 0.99 in mass fraction) and absolute ethanol (> 0.99 in mass fraction) were purchased from Merck.

Apparatus and Procedures. The binary mixtures of ethanol + 2,2,4-trimethylpentane were prepared with appropriate mass fractions. The mole fractions of the solvents were computed with the uncertainty of 0.001. The solubility of the analytes was determined by equilibrating excess amounts of the solids with the binary solvent mixtures using a shaker (Behdad, Tehran, Iran) placed in an incubator equipped with a temperature controlling system at (298.2, 308.2, and 318.2) ± 0.2 K (Nabziran, Tabriz, Iran). For assurance of equilibrium, samples were incubated for three days at 298.2 K. After solubility determination and density measurement at 298.2 K, the remaining solutions containing excess solid were placed at 308.2 K for 1 day, and the measurements were carried out; the same procedure was repeated for 318.2 K. The sample solutions were filtered using hydrophobic Durapore filters (0.45 μm, Millipore, Ireland) and then were diluted using appropriate solvents (methanol for anthracene and 2-propanone for phenanthrene) for spectrophotometric analyses. Absorbances of the diluted solutions were recorded at 356 nm (for anthracene) and 345 nm (for phenanthrene) using a UV–vis spectrophotometer (Beckman DU-650, Fullerton, USA). Molar concentrations of the diluted solutions were determined from UV absorbance calibration graphs. The molar absorptivities of anthracene ranging from $\epsilon = 8177 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ to $\epsilon = 8199 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ for compositions ranging from 0.000028 mol·L^{−1} to 0.000210 mol·L^{−1}. The molar

Table 2. Details of Different Numerical Methods Using the Jouyban–Acree Model Employed in This Study

method	J terms	solubilities in monosolvent
I	fitted parameters from eq 1 using solubility data at each temperature	experimental
II	fitted parameters from eq 1 using solubility data at 298.2 K	experimental
III	eqs 2 to 4	experimental
IV	eqs 5 to 7	experimental
V	eqs 8 to 10	experimental

absorptivities of phenanthrene ranging from $\varepsilon = 243 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ to $\varepsilon = 224 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ for compositions ranging from $0.002244 \text{ mol} \cdot \text{L}^{-1}$ to $0.005611 \text{ mol} \cdot \text{L}^{-1}$. Densities of the saturated solutions were determined using a 5 mL pycnometer.

CALCULATIONS

Computing the Model Constants of Solutes in Ethanol + 2,2,4-Trimethylpentane. The generated experimental solubility data of anthracene and phenanthrene in ethanol + 2,2,4-trimethylpentane at various temperatures were separately fitted to eq 1, and the model constants were calculated by regressing $(\ln X_{m,T}^{\text{Sat}} - x_1 \ln X_{1,T}^{\text{Sat}} - x_2 \ln X_{2,T}^{\text{Sat}})$ against $((x_1 \cdot x_2)/T)$, $((x_1 \cdot x_2 (x_1 - x_2))/T)$, and $((x_1 \cdot x_2 (x_1 - x_2)^2)/T)$. Then the calculated solubility data were used to compute the mean relative deviations (MRD) as a criterion of error by

$$\text{MRD} = \frac{1}{N} \sum \left[\frac{|(X_m^{\text{Sat}})_{\text{pred}} - (X_m^{\text{Sat}})_{\text{exp}}|}{(X_m^{\text{Sat}})_{\text{exp}}} \right] \quad (11)$$

in which N is the number of data points in each set. This numerical analysis was called method I.

Predicting the Solubility of Solutes in Ethanol + 2,2,4-Trimethylpentane at (308.2 and 318.2) K. The generated experimental solubility data of anthracene and phenanthrene in ethanol + 2,2,4-trimethylpentane at 298.2 K were separately fitted to eq 1, and the trained models were used to predict the solubility of solutes at (308.2 and 318.2) K, employing the solubility data in monosolvents at these temperatures. Then the MRDs for predicted data points were calculated using eq 11. This analysis is called method II.

Predicting the Solubility of Solutes in Ethanol + 2,2,4-Trimethylpentane at Various Temperatures Using Hildebrand Solubility Parameters. By using eqs 2 to 4, J_i terms of the Jouyban–Acree model for binary solvent mixtures were calculated. The obtained model was used to predict the solubility of solutes at (298.2, 308.2, and 318.2) K, employing the solubility data in monosolvents at these temperatures. Then the MRDs for predicted data points were calculated using eq 11. This analysis is called method III.

Predicting the Solubility of Solutes in Ethanol + 2,2,4-Trimethylpentane at Various Temperatures Using Abraham Parameters. By using eqs 5 to 7, J_i terms of the Jouyban–Acree model for binary solvent mixtures were calculated. The trained model was used to predict the solubility of solutes at (298.2, 308.2, and 318.2) K, employing the solubility data in monosolvents at these temperatures. Then the MRDs for predicted

Table 3. Solvent Composition (in Mole Fraction), Density ρ of Saturated Solutions, and Experimental Mole Fraction Solubility of Anthracene ($10^{-5} X_{T,\text{exp}}^{\text{Sat}}$) and Phenanthrene (X_m^{Sat}) in Binary Ethanol + 2,2,4-Trimethylpentane Mixtures

mole fraction	$10^{-5} X_{T,\text{exp}}^{\text{Sat}}$ (mole fraction)	density ρ ($\text{g} \cdot \text{cm}^{-3}$)	$X_{T,\text{exp}}^{\text{Sat}}$ (mole fraction)	density ρ ($\text{g} \cdot \text{cm}^{-3}$)
Anthracene				
$T = 298.2$				
0.000	118.7	0.684	0.0246	0.693
0.239	127.7	0.691	0.0272	0.705
0.414	114.3	0.701	0.0266	0.718
0.548	104.1	0.710	0.0239	0.726
0.653	95.0	0.720	0.0220	0.738
0.739	88.5	0.730	0.0213	0.746
0.809	82.1	0.742	0.0196	0.757
0.868	74.2	0.751	0.0171	0.767
0.919	67.3	0.761	0.0149	0.777
0.962	60.8	0.769	0.0134	0.787
1.000	50.5	0.776	0.0119	0.793
$T = 308.2$				
0.000	151.5	0.679	0.0378	0.706
0.242	161.0	0.687	0.0385	0.726
0.418	146.6	0.697	0.0388	0.736
0.552	135.9	0.706	0.0347	0.748
0.657	124.4	0.716	0.0320	0.756
0.742	116.0	0.726	0.0298	0.766
0.812	105.9	0.736	0.0273	0.776
0.870	95.9	0.746	0.0234	0.786
0.920	86.2	0.755	0.0212	0.796
0.963	77.7	0.765	0.0181	0.806
1.000	66.5	0.777	0.0159	0.812
$T = 318.2$				
0.000	176.8	0.679	0.0484	0.720
0.240	189.8	0.687	0.0510	0.734
0.415	170.5	0.697	0.0473	0.744
0.549	154.8	0.706	0.0421	0.758
0.654	140.4	0.716	0.0384	0.768
0.739	129.5	0.726	0.0358	0.778
0.810	121.4	0.736	0.0322	0.792
0.869	108.7	0.746	0.0282	0.796
0.919	97.9	0.755	0.0254	0.812
0.962	88.4	0.767	0.0227	0.814
1.000	78.0	0.775	0.0190	0.816

data points were calculated using eq 11. This analysis is called method IV. Similar procedures could be used to develop a predictive method employing the experimental data in monosolvents and J terms calculated using eqs 8 to 10 (method V). The Abraham solute parameters for anthracene are $E = 2.290$, $S = 1.34$, $B = 0.280$, $V = 1.4540$, and $L = 7.568$, and those of phenanthrene are $E = 2.055$, $S = 1.29$, $B = 0.29$, $V = 1.4544$, and $L = 7.632$.¹¹ A summary of methods I to V is listed in Table 2.

Predicting the Density of Saturated Solutions at Various Temperatures Using a Trained Model for Ethanol + 2,2,4-

Table 4. Solubility of Anthracene and Phenanthrene in Ethanol and 2,2,4-Trimethylpentane at 298.2 K Taken from the Literature and the Generated Data in This Work

solute	solvent	solubility (unit)	reference	solubility (unit)	reference	difference %
anthracene	ethanol	0.0078 (mol·L ⁻¹)	10	0.0085 (mol·L ⁻¹)	this work	-8.2
anthracene	ethanol	0.0087 (mol·L ⁻¹)	16	0.0085 (mol·L ⁻¹)	this work	2.4
anthracene	2,2,4-trimethylpentane	0.0066 (mol·L ⁻¹)	10	0.0071 (mol·L ⁻¹)	this work	-7.0
anthracene	2,2,4-trimethylpentane	0.0067 (mol·L ⁻¹)	16	0.0071 (mol·L ⁻¹)	this work	-5.6
phenanthrene	ethanol	0.0128 (mole fraction)	17	0.0119 (mole fraction)	this work	7.6
phenanthrene	ethanol	0.0111 (mole fraction)	18	0.0119 (mole fraction)	this work	-6.7
phenanthrene	ethanol	0.0111 (mole fraction)	8	0.0119 (mole fraction)	this work	-6.7

Table 5. The Jouyban–Acree Model Constants Calculated for Studied Solutes in Ethanol + 2,2,4-Trimethylpentane Solvent Mixtures

solute	J_0	J_1	J_2
anthracene	382.630	86.985	432.112
phenanthrene	456.829	171.041	307.215

Table 6. The Mean Relative Deviation (MRD) for Numerical Methods I to V for Predicting Solubility of Anthracene and Phenanthrene in Ethanol + 2,2,4-Trimethylpentane Mixtures

solute	I	II	III	IV	V
anthracene	1.1	1.4	11.8	6.8	27.6
phenanthrene	1.5	1.9	14.2	4.4	24.6

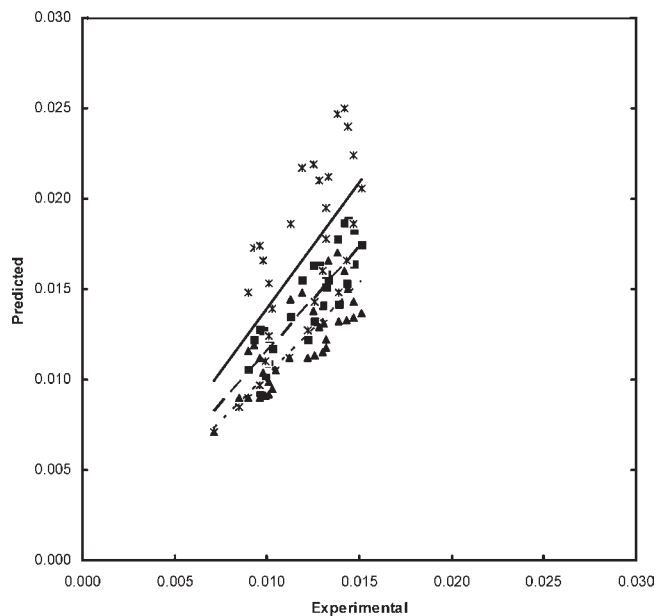
Trimethylpentane Mixtures. By using the solute free density data of ethanol + 2,2,4-trimethylpentane mixtures at various temperatures, the Jouyban–Acree model could be trained as¹³

$$\ln \rho_{m,T} = x_1 \ln \rho_{1,T} + x_2 \ln \rho_{2,T} - 49.137 \left(\frac{x_1 x_2}{T} \right) + 12.03 \left(\frac{x_1 x_2 (x_1 - x_2)}{T} \right) \quad (12)$$

in which $\rho_{m,T}$ is the density of mixed solvent system in the absence of a solute and $\rho_{1,T}$ and $\rho_{2,T}$ are the density of monosolvents 1 and 2 in the absence of a solute at temperature of T . This model was used to predict the density of saturated solutions at various temperatures.

RESULTS AND DISCUSSION

Mole fraction compositions of the binary solvent mixtures, solubilities of anthracene and phenanthrene, densities of the solute free mixed solvents, and the density of saturated solutions at different temperatures are reported in Table 3. Each experimental data point is an average of at least three experimental measurements with the measured mol·L⁻¹ solubilities being reproducible to within $\pm 2.7\%$ and 2.5% and standard deviations ranging from ($\sigma_{n-1} = 0.00065$ to $\sigma_{n-1} = 0.00010$) mol·L⁻¹ and from ($\sigma_{n-1} = 0.0002$ to $\sigma_{n-1} = 0.0250$) mol·L⁻¹, respectively, for anthracene and phenanthrene. The reported solubility data of the solutes from the literature are listed in Table 4. There are good agreements between generated solubility data in this work with those from the literature. The J_i terms of the Jouyban–Acree model for studied solutes in ethanol + 2,2,4-trimethylpentane solvent mixtures were calculated using a no-intercept regression analysis and are listed in Table 5. The MRD values for the predicted solubility using different numerical methods

**Figure 2.** Predicted solubility of anthracene using different numerical analyses versus experimental values; method III, \blacktriangle , - - -; method IV, \blacksquare , - - -; and method V, *, —.

for anthracene and phenanthrene were tabulated in Table 6. The results showed that the Jouyban–Acree model is well fitted to the generated data with MRD values of 1.1 % and 1.5 %, respectively, for anthracene and phenanthrene (method I). The trained model using solubility data at a constant temperature (i. e., 298.2 K) can be used to predict the solubility at other temperatures ((308.2 and 318.2) K) in which the MRD values of 1.4 % and 1.9 % were obtained for anthracene and phenanthrene. The solubility prediction capability of anthracene and phenanthrene at different temperatures using previous trained models at constant temperatures (methods III to V) are 11.8, 6.8, 27.6, and 14.2, 4.4, and 24.6, respectively. Figure 2 illustrated the predicted solubility of anthracene in ethanol + 2,2,4-trimethylpentane at different temperatures using methods III to V. The correlation coefficients of methods III to V are 0.7773, 0.7949, and 0.7078, respectively. The closer correlation coefficient to 1.0000 means more accurate predicted solubilities by the method, and concerning this, method IV provided the best predictions followed by methods III and V. The slope of the no-intercept linear equation between predicted and experimental values could be considered as another criterion. The slopes for methods III, IV, and V are 1.0211, 1.1548, and 1.3967, respectively, in which the ideal value for the slope is 1.0000. Considering this criterion, prediction performance of the method III is better than method

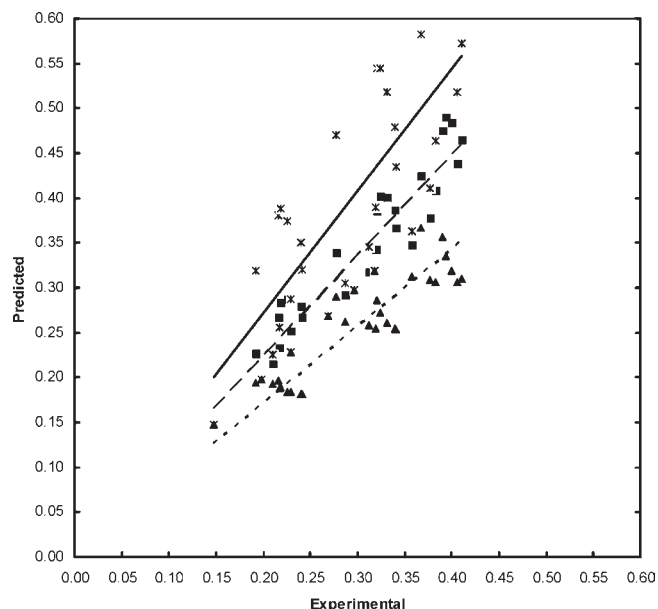


Figure 3. Predicted solubility of phenanthrene using different numerical analyses versus experimental values; method III, \blacktriangle , - - -; method IV, \blacksquare , —; and method V, *, —.

IV, followed by method V. A similar plot for phenanthrene data was shown in Figure 3, in which the correlation coefficients for methods III, IV, and V are 0.8800, 0.9465, and 0.8076, respectively. The corresponding slopes are 0.8572, 1.1184, and 1.3620. These findings are in agreement with the MRD values reported in Table 6. These results show that trained model using water to solvent Abraham coefficient (method IV) provide more accurate predictions for the reported solubility data in this study.

The densities of the solute saturated solution were predicted using eq 12 and experimental $\rho_{1,T}$ and $\rho_{2,T}$ of the saturated solutions. The results show that MRD values of eq 12 for predicting densities of anthracene and phenanthrene in ethanol + 2,2,4-trimethylpentane mixtures at various temperatures are 0.5 % and 0.9 %, respectively.

As a conclusion, the solubility prediction of drugs and chemical compounds such as PAHs in solvent mixtures at different temperatures is very important in chemical and pharmaceutical sciences. Solubilities of two PAHs were reported in a binary solvent mixture at various temperatures, and the results of the numerical analyses revealed that previous QSPR models can be extended to solubility prediction at different temperatures.

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