Solubility of Fluorene in Different Solvents from 278.98 K to 338.35 K

Zhan Zou,* Leping Dang, Pengbiao Liu, and Hongyuan Wei

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Using a laser monitoring observation technique, the solubility of fluorene in dimethylbenzene, methylbenzene, ethanol, isopropanol, and *n*-butanol from 278.98 K to 338.35 K was experimentally measured by a synthetic method. The results were correlated with a semiempirical equation and provided an indication of the solution nonidealities on the solubility of the solute, which can be used as a useful model in the production of fluorene.

Introduction

Fluorene (CAS No.: [86-73-7]) is one of the polycyclic aromatic hydrocarbons, which is purified from coal tar.[1,2] It is a white or almost white powdered crystal, and the chemical structure is shown in Figure 1. Fluorene is an important material

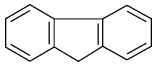

Figure 1. Molecular structure of fluorene.

in organic synthesis, the pharmacy industry, the synthetic resin industry, and so on. The entire usage required purified fluorene. So, it is necessary to measure the solubility of fluorene in different solvents. However, no experimental solubility data were available in the literature until now. In this work, the solubility of fluorene in dimethylbenzene, methylbenzene, ethanol, isopropanol, and *n*-butanol was experimentally determined using a laser monitoring observation technique.[3,4]

Experimental Section

A white crystalline powder of fluorene with a melting point of (116 ± 0.5) °C was used, and its purity is higher than 99.5 mass %. The solvents including dimethylbenzene, methylbenzene, ethanol, isopropanol, and *n*-butanol (purchased from Tianjin Kewei Co. of China) were of analytical reagent grade, and their purity was higher than 99.8 mass %.

The solubility of fluorene in different solvents was measured by a synthetic method which is described in the literature.[5−8] All the experiments were conducted three times, and the mean values were used to calculate the mole fraction solubility x_1. The uncertainty of the experimental solubility values is within 0.0200.[9−11]

Results and Discussion

The solubilities of fluorene in dimethylbenzene, methylbenzene, ethanol, isopropanol, and *n*-butanol at different temperatures are listed in Table 1. x_1^{exptl} expresses the experimental value of solubility, and RD is defined as follows

$$RD = \frac{x_1^{exptl} - x_1^{calcd}}{x_1^{exptl}} \quad (1)$$

* Corresponding author. Phone: +86 (0)22 27405754. Fax: +86 (0)22 27400287. E-mail: zouzhan999@hotmail.com.

Table 1. Mole Fraction Solubility Data of Fluorene in Different Solvents

T/K	$10^2 \cdot x_1^{exptl}$	RD %	*T*/K	$10^2 \cdot x_1^{exptl}$	RD %
		Dimethylbenzene			
283.21	1.814	−0.727	308.15	9.015	−0.922
289.11	2.685	−0.828	313.67	12.71	−0.250
293.18	3.495	−1.070	318.83	17.43	0.449
298.62	4.982	−0.575	323.17	22.59	0.809
303.67	6.897	0.090	328.45	30.30	−0.431
		Methylbenzene			
283.27	6.341	−0.823	308.81	20.05	0.597
288.77	8.185	−0.360	314.04	25.21	1.040
293.72	10.19	−0.713	319.01	30.77	−0.123
298.89	12.95	0.221	323.28	36.71	−0.394
303.17	15.45	−0.948			
		Ethanol			
278.98	0.372	0.101	303.36	0.973	0.828
283.99	0.455	0.155	308.77	1.185	−0.027
289.01	0.554	0.127	313.17	1.387	−0.862
294.08	0.668	−0.992	319.27	1.766	0.556
298.35	0.802	0.706	324.95	2.161	−0.193
		Isopropanol			
288.28	0.221	−0.052	313.78	1.047	−0.414
293.69	0.313	0.224	318.24	1.355	−0.223
299.50	0.453	0.893	323.17	1.787	−0.230
303.17	0.565	0.690	328.25	2.368	0.009
309.06	0.802	0.496	333.45	3.136	0.079
		n-Butanol			
284.27	0.590	−1.512	313.93	2.122	0.574
288.82	0.724	−1.102	318.16	2.510	0.250
293.76	0.906	−0.055	323.16	3.038	−0.626
298.88	1.130	0.123	328.25	3.703	−0.873
304.06	1.390	−0.998	333.35	4.578	0.534
308.28	1.679	0.323	338.35	5.584	1.221

Table 2. Parameters of the Apelblat Equation for Fluorene in Different Solvents

solvents	*A*	*B*	*C*	10^3rmsd
dimethylbenzene	−102.22	−405.55	17.649	0.821
methylbenzene	−103.82	1180.4	17.162	1.231
ethanol	−102.96	1448.2	16.369	0.063
isopropanol	−68.045	−1896.3	12.096	0.031
n-butanol	−88.212	508.85	14.390	0.268

where x_1^{calcd} expresses the calculated value of solubility. This variable can be computed by the Apelblat equation as follows

$$\ln x = A + \frac{B}{T} + C \cdot \ln T \quad (2)$$

where *A*, *B*, and *C* are empirical constants.

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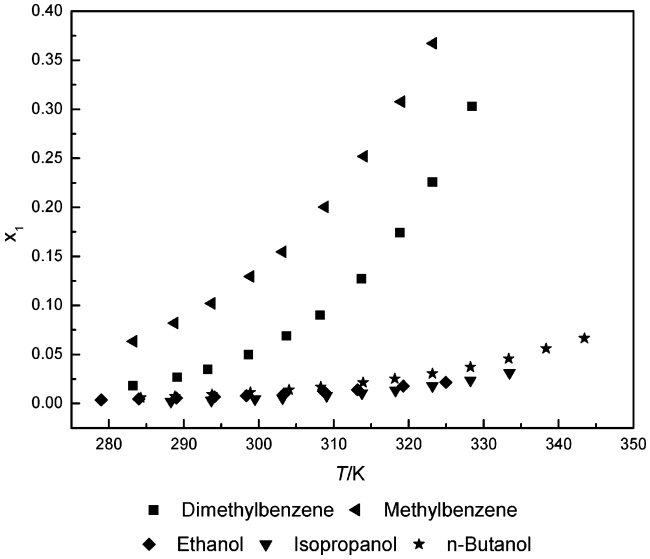

Figure 2. Solubility of fluorene in different solvents.

The experimental solubility values were correlated with eq 2 in the least-squares method, and the difference between experimental and calculated results is presented in Table 1. The values of the three parameters, *A*, *B*, and *C*, together with the root-mean-square deviations (rmsd) are listed in Table 2. The rmsd is defined as the following

$$\text{rmsd} = \left[\frac{1}{N}\sum_{i=1}^{n}(x_i^{\text{exptl}} - x_i^{\text{calcd}})^2\right]^{1/2} \quad (3)$$

where *N* is the number of experimental points.[10−12]

Conclusions

From Tables 1 and 2 and Figure 2, we can draw the following conclusions: (1) The solubility of fluorene in dimethylbenzene, methylbenzene, ethanol, isopropanol, and *n*-butanol is a function of temperature, and it increases with the increase of temperature. (2) The solubility of fluorene increases with the solvents in the order: isopropanol, ethanol, *n*-butanol, dimethylbenzene, methylbenzene. (3) The calculated solubility of fluorene sets a good coherence with the experimental values, and the experimental solubility and correlation equation in this work can be used as essential data and models in the research and crystallization of fluorene.

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