Solubility of Acenaphthylene in Different Solvents between (278 and 323) K

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The solubility of acenaphthylene in different solvents (methylbenzene, 1-butanol, 2-propanol, and ethanol) was measured using a synthetic method at temperatures ranging from (278 to 323) K at atmospheric pressure. The experimental data were correlated with the Apelblat equation. The results should be useful for the industrial crystallization of acenaphthylene.

Introduction

Acenaphthylene(1,8-dihydroacenaphthalene) is a white crystal with a melting point of (95 ± 0.5) °C. In organic synthesis, acenaphthylene is an important intermediate material, which is widely used for the synthesis of advanced pigments, dyes, and polymers.[1] The entire usage requires purified acenaphthylene products. Crystallization processes are the critical steps that determine the quality of the final product. The solubility of solid compounds in solvents plays a crucial role in the development and operation of crystallization processes. Therefore, knowing the solubility of the product is necessary. The published works relating to acenaphthylene are mainly concerned with synthesis. Literature on the solubility of acenaphthylene in common solvents is scarce.

In the present work, the solubility of acenaphthylene in methylbenzene, 1-butanol, 2-propanol, and ethanol was measured in the temperature range from (278.00 to 323.00) K by a laser monitoring observation technique.[2,3]

Experimental

A white crystalline powder of acenaphthylene was used, and its mass fraction purity was higher than 99.5 %. The solvents including methylbenzene, 1-butanol, 2-propanol, and ethanol (purchased from Tianjin Kewei Co. of China) were of analytical reagent grade, and their mass fraction purity was higher than 99.8 %. The solubility was measured by a synthetic method which is described in the literature.[4−6] All the experiments were conducted three times, and the relative uncertainty of the experimental solubility values is within 0.0200. The mean values were used to calculate the mole fraction solubility x_1.

Results and Discussion

The solubilities of acenaphthylene in methylbenzene, 1-butanol, 2-propanol, and ethanol at different temperatures are listed in Table 1 and plotted in Figure 1. x_1 is the experimental value of solubility. x_1^{calcd} expresses the calculated value of solubility. This variable can be computed by the Apelblat equation[7] as follows

$$\ln x_1^{\text{calcd}} = A + \frac{B}{T/\text{K}} + C \ln T/\text{K} \qquad (1)$$

where A, B, and C are empirical constants.

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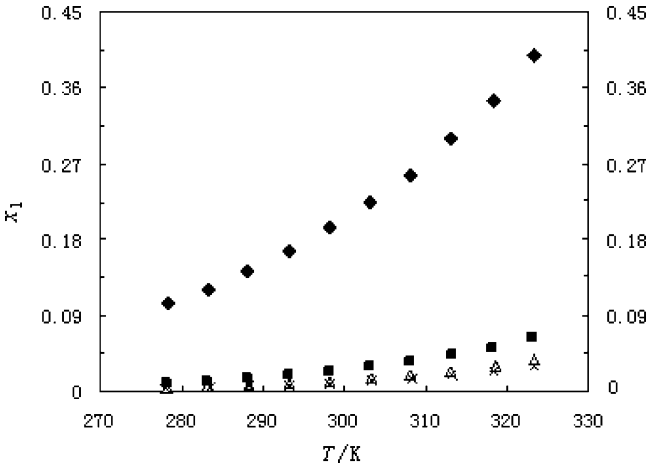

Figure 1. Solubility x_1 of acenaphthylene in different solvents: ◆, methylbenzene; ■, 1-butanol; △, 2-propanol; ×, ethanol.

Table 1. Mole Fraction Solubility x_1 of Acenaphthylene in Different Solvents

T/K	10^2x_1	$(x_1 - x_1^{calcd})/x_1$	T/K	10^2x_1	$(x_1 - x_1^{calcd})/x_1$
		Ethanol			
278.10	0.4622	0.0121	303.20	1.3276	−0.0063
283.53	0.5785	−0.0038	308.20	1.6519	0.0093
288.25	0.7093	−0.0051	313.05	1.9700	−0.0083
293.25	0.8913	0.0095	318.25	2.4486	0.0049
298.20	1.0793	−0.0069	323.15	2.9553	0.0036
		2-Propanol			
278.30	0.4687	0.0034	303.30	1.5233	−0.0097
283.07	0.5923	0.0010	308.05	1.8871	−0.0095
288.33	0.7701	0.0079	312.95	2.3581	−0.0035
293.20	0.9671	0.0036	318.40	3.0246	0.0086
298.07	1.1972	−0.0107	323.25	3.7196	0.0085
		1-Butanol			
278.25	1.0098	0.0054	303.15	2.8995	0.0081
283.05	1.2221	−0.0120	308.10	3.4855	−0.0090
288.05	1.5448	0.0082	313.20	4.2705	−0.0106
293.25	1.8975	−0.0058	318.05	5.2492	0.0036
298.25	2.3672	0.0069	323.05	6.3929	0.0049
		Methylbenzene			
278.47	10.417	−0.0033	303.15	22.391	0.0011
283.33	12.178	−0.0021	307.95	25.590	−0.0062
288.10	14.175	0.0002	312.95	29.854	0.0035
293.15	16.702	0.0085	318.30	34.574	−0.0017
298.23	19.355	0.0020	323.20	39.835	0.0030

The experimental solubility values were correlated with eq 1 by a 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

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

solvents	*A*	*B*	*C*	100·mrd
ethanol	−73.395	−83.508	12.137	0.697
2-propanol	−71.517	−515.22	12.081	0.665
1-butanol	−93.112	844.83	15.186	0.746
methylbenzene	−53.186	21.255	9.033	0.315

mean relative deviations (mrd) are listed in Table 2. The mrd is defined as the following

$$\mathrm{mrd} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{x_1 - x_1^{\mathrm{calcd}}}{x_1}\right| \qquad (2)$$

where N is the number of experimental points.

Conclusions

From Tables 1 and 2 and Figure 1, we can draw the following conclusions: (1) The solubility of acenaphthylene in methylbenzene, 1-butanol, 2-propanol, and ethanol is a function of temperature, and it increases with the increase of temperature. (2) The solubility of acenaphthylene increases with the solvents in the order: methylbenzene, 1-butanol, 2-propanol, and ethanol.

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