Solubility of Acenaphthene in Different Solvents from (283.00 to 323.00) K

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The solubility of acenaphthene in benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol was experimentally measured at temperatures ranging from (283.00 to 323.00) K. The laser monitoring observation technique was used to determine the disappearance of the solid phase in a solid + liquid mixture. The results of these measurements were correlated with the Apelblat equation.

Introduction

Acenaphthene is a white needle-like crystal. In organic material industry, acenaphthene has received great attention, which is being investigated and developed for use as an electro-optical device and photoconductor materials.[1,2] In the final purification step, acenaphthene is often refined through cooling crystallization from solution. The determination of its solubility in different solvents is crucial to choose the proper solvent and to optimize the crystallization process. Therefore, knowing the solubility of the product is necessary. Choi et al. determined the solubility of acenaphthene in benzene and in mixtures of benzene and cyclohexane.[3] Thenmozhi et al. measured the solubility of acenaphthene in nonaqueous solvents at the temperature of (298.15 to 333.15) K.[4] In their studies, the mass fraction purity of acenaphthene used was about 99.0 %. Especially, acenaphthene used was not purified in the Choi work. In this work, the solubility of acenaphthene (mass fraction purity 99.85 %) in benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol has been measured.

In this paper, the solubility of acenaphthene in benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol was experimentally measured from (283.00 to 323.00) K using a laser monitoring observation technique.[5,6]

Experimental Section

Acenaphthene was recrystallized more than three times from ethanol by cooling crystallization. A white and needle-like crystal of acenaphthene was used during the experiment. Its purity was analyzed by gas chromatography, and its melting point was determined by differential scanning calorimetry. The results were as follows: purity, 99.85 %; melting point, 368 K. The solvents used including benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol (purchased from the 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 the method which is described in the literature.[7−9] All the experiments were conducted three times, and the mean values were used to calculate the mole fraction solubility x_1 of acenaphthene in benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol. The relative uncertainty of the experimental solubility values is within 0.02.

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Table 1. Mole Fraction Solubility of Acenaphthene (x_1) in Benzene, 1,3-Dimethylbenzene, Acetone, 1-Propanol, and Isobutanol from (283.00 to 323.00) K

T/K	10^2x_1	$[100(x_1 - x_1^{calc})]/x_1$	T/K	10^2x_1	$[100(x_1 - x_1^{calc})]/x_1$
acetone			1,3-dimethylbenzene		
283.00	4.168	7.09	283.00	10.86	−1.02
288.00	4.911	4.73	288.00	12.91	2.75
293.00	5.867	3.83	293.00	14.32	−0.85
298.00	6.920	1.89	298.00	16.28	−0.92
303.00	7.881	−3.46	303.10	18.83	0.22
308.10	9.545	−2.78	308.20	21.64	−0.07
313.00	11.32	−3.33	313.00	24.54	−0.07
318.00	13.58	−2.86	318.00	28.05	−0.06
323.00	17.26	3.55	323.00	32.10	0.14
isobutanol			1-propanol		
283.00	0.926	−10.1	283.00	0.879	−4.11
288.10	1.282	0.77	288.10	1.198	5.90
293.20	1.618	2.09	293.20	1.443	3.92
298.00	2.046	4.92	298.00	1.752	4.01
303.30	2.529	3.72	303.30	2.075	−0.23
308.00	2.975	0.28	308.00	2.457	−2.08
313.10	3.533	−3.84	313.10	2.951	−3.99
318.00	4.345	−3.41	318.00	3.640	−2.19
323.00	5.650	2.38	323.00	4.643	2.64
benzene					
283.00	11.80	3.93			
288.00	13.12	1.91			
293.20	14.24	−3.06			
298.00	16.23	−2.15			
303.00	18.73	−0.50			
308.30	21.48	−0.21			
313.00	24.37	0.49			
318.00	27.69	0.59			
323.00	31.21	−0.10			

Results and Discussion

The solubilities of acenaphthene in benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol at different temperatures are listed in Table 1. Compared with this work, the solubilities reported by Thenmozhi and Choi are about 10 % bigger. So, it is suggested that the impurities could play an important role. Further discussion of the effect of impurities on solubility of acenaphthene in these organic solvents is complicated and beyond the scope of this article.

This variable can be computed by the Apelblat equation[10] as follows

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$$\ln x = A + \frac{B}{T/\mathrm{K}} + C \ln(T/\mathrm{K}) \quad (1)$$

The experimental solubility values were correlated with eq 1 using the least-squares method, and the difference between experimental and calculated results is presented in Table 1. x_1^{calc} represents the solubility calculated from eq 1, and x_1 represents the experimental solubility values. The values of the three parameters, A, B, and C, together with the root-mean-square relative deviations (rmsd), are listed in Table 2. The rmsd is defined as the following

$$\mathrm{rmsd} = \left\{ \frac{1}{N} \sum_{i=1}^{N} \left(\frac{x_i^{calc} - x_i}{x_i} \right)^2 \right\}^{1/2} \quad (2)$$

where N is the number of experimental points.

The fractional deviations $\Delta x = (x_1 - x_1^{calc})/x_1$ of the experimental solubility x_1 of acenaphthene in benzene from values x_1^{calc} obtained with the correlation of the Apelblat equation in this work, in ref 3 and in ref 4, are plotted in Figure 1. From Figure 1, it can be seen that the fractional deviations are smaller in this work than that in ref 3 and in ref 4.

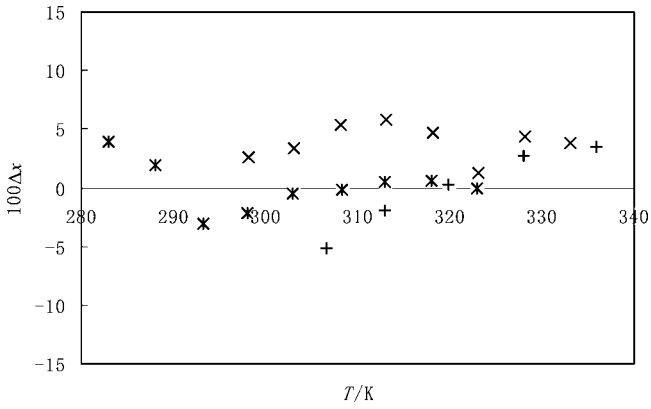

Figure 1. Fractional deviations $\Delta x = (x_1 - x_1^{calc})/x_1$ of the experimental solubility x_1 of acenaphthene in benzene from values x_1^{calc} obtained with the correlation of the Apelblat equation. *, in this work; +, in ref 3; ×, in ref 4.

Table 2. Curve-Fitting Parameters of Equation 2 for Acenaphthene in Benzene, 1,3-Dimethylbenzene, Acetone, 1-Propanol, and Isobutanol from (283.00 to 323.00) K

solvent	A	B	C	100 rmsd
benzene	−97.110	2325.1	15.36	1.94
1,3-dimethylbenzene	−96.963	2203.5	15.404	1.07
acetone	−91.880	1185.9	14.956	3.98
1-propanol	−120.83	2156.6	19.222	3.58
isobutanol	−119.32	1918.2	19.123	4.43

Conclusions

From Tables 1 and 2, we can draw the following conclusions: (1) The solubility of acenaphthene in benzene, 1,3-dimethylbenzene, acetone, 1-propanol, and isobutanol is a function of temperature, and it increases with an increase in temperature. (2) The mole fraction solubility of acenaphthene in benzene and 1,3-dimethylbenzene is near and more than that of acenaphthene in acetone, isobutanol, and 1-propanol. The solubility increases with the solvents in the order: acetone, isobutanol, 1-propanol. (3) The calculated solubility of acenaphthene sets a good coherence with the experimental values, and the experimental solubility and correlation equation in this work can be used for solvent selection and model research of the crystallization process of acenaphthene.

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