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Thermodynamic properties of disodium sebacate in different binary solvent mixtures

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ABSTRACT

The solubility data of disodium sebacate in three kinds of water + organic solvent mixtures, including (water + methanol), (water + acetone) and (water + DMF), were experimentally determined at temperatures from (283.15 to 328.15) K by a gravimetric method. The results show that the solubility of disodium sebacate increases with increase of temperature in binary solvent mixtures at constant solvent composition, whereas it decreases with the increase of the mole fraction of organic solvent. The modified Apelblat equation, the λ*h* model and the NRTL model were applied to correlate the solubility data in binary solvent mixtures. In addition, the dissolution thermodynamic properties of disodium sebacate in different binary solvent mixtures, including the Gibbs energy change, entropy and enthalpy, were also calculated and discussed based on the NRTL model and experimental solubility data.

1. Introduction

Disodium sebacate (NaOOC-$(CH_2)_8$-COONa, CAS No. 17265-14-4) is a white powdered crystal and is generated in cracking process and then acidified to sebacic acid, which is extremely valuable for the production of nylon, alkyd resins, plasticizers, cosmetics, and biological agents, and so forth [1–4].

Generally, the acidization from disodium sebacate to sebacic acid is processed in water. Since the solubility of sebacic acid in water is pretty low and is prone to cause outbreak of nucleation and serious agglomeration, which will result in decanedioic acid product with small size product and uneven size distribution. Usually, decanedioic acid product with larger size and more homogeneous particle distribution will be favorite since their easier downstream processing, such as filtration, drying, and packing. As we all know, the solvent could significantly affect the crystallization process and therefore will affect the quality of final product. To overcome the burst of nucleation during acidization in water, acidization in binary solvent mixtures of water and organic solvents is one possible solution. Therefore, it is important to know the solid-liquid equilibrium data [5] of disodium sebacate in binary solvent mixtures.

Apart from the effects of NaOH and ethanol on the solubility of disodium decanedioate in water studied by Qing Xia's group [6], the solubility of disodium sebacate has not been reported in the literature. In this work, the solubilities of disodium sebacate in water + organic solvent mixtures at different temperatures were measured by a gravimetric method in a temperature range from (283.15 to 328.15) K. Different models were used to correlate the experimental solubility data. The dissolution thermodynamic properties were also investigated.

2. Experimental

2.1. Materials

Disodium sebacate was supplied by TongTuo chromatographic technology Co., Ltd. (Tianjin, China). The organic solvents, including methanol, acetone and DMF were provided by Tianjin Guangfu Chemical Technique Co., Ltd. (Tianjin, China). Distilled–deionized water was supplied by Nankai University, China. All chemicals were used without further purification. More detailed information about the materials used in this work has been listed in Table 1.

2.2. Characterization

The solid state samples in the experiments were analyzed by X-ray powder diffraction [7] (type D/max-2500, Rigaku, Japan) and differential scanning calorimetry (DSC 1/500, Mettler-Toledo, Switzerland) [8] before and after the dissolution of disodium sebacate in the tested solvents. X-ray powder diffraction was used

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Table 1
Sources and mass fraction purity of materials.

Chemical name	Source	Mass fraction purity	Purification method	Analysis method
Disodium sebacate	TongTuo chromatographic technology	>0.99	None	HPLC[a]
Methanol	Tianjin Guangfu Chemical	>0.995	None	GC[b]
Acetone	Tianjin Guangfu Chemical	>0.995	None	GC[b]
DMF	Tianjin Guangfu Chemical	>0.995	None	GC[b]

Both the analysis method and the mass fraction purity were provided by the suppliers.
[a] High-performance liquid chromatography.
[b] Gas chromatography.

to identify the crystal over a diffraction-angle range of 2° to 50°, at a scanning rate of $0.10°\cdot s^{-1}$. The melting temperature T_{melt} and enthalpy of fusion $\Delta_{fus}H$ of disodium sebacate were measured by DSC under nitrogen atmosphere.

2.3. Solubility measurements by gravimetric method

The solubility of disodium sebacate in different binary solvent mixtures was determined by the gravimetric method which was described in the literature [9,10]. At first, an excess amount of disodium sebacate powder was added into the solvent mixtures. The solution was stirred in a 50 ml jacketed glass vessel for 8 h, the preliminary experiments proved that 8 h are enough for this system to reach solid-liquid equilibrium. Then the agitation was stopped and the suspension was kept static for 6 h to make sure the undissolved particles settle down. After that, the upper clear saturated solutions were withdrawn and filtered by an organic membrane (0.2 μm) filter and dried in a vacuum oven at 313.15 K for 20 h. The temperature of the glass vessel was controlled by a thermostat (Julabo CF41, Germany) with an accuracy of ± 0.02 K. All the masses were measured by an analytical balance (Mettler ToledoML204, Switzerland). The process was repeated three times for each solubility point. Then the mean values were used to calculate the mole fraction solubility.

The mole fraction solubility (x_1) of disodium sebacate in binary solvent mixtures was calculated by using Eq. (1), and the initial mole fraction (x_2) of water in the binary solvent mixtures is expressed by Eq. (2):

$$x_1 = \frac{m_1/M_1}{m1/M_1 + m2/M_2 + m_3/M_3} \quad (1)$$

$$x_2 = \frac{m_2/M_2}{m_2/M_2 + m_3/M_3} \quad (2)$$

where m_1, m_2 and m_3 represent the mass of solute (disodium sebacate), water and organic solvent (methanol, acetone or DMF) respectively. M_1, M_2 and M_3 are the corresponding molecular mass of them.

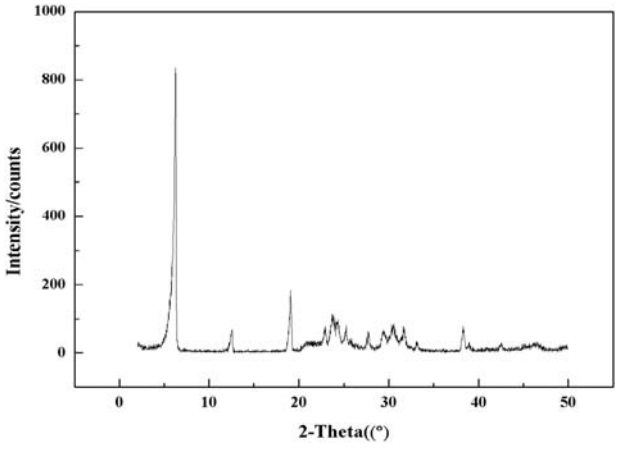

Fig. 1. X-ray powder diffraction pattern of disodium sebacate.

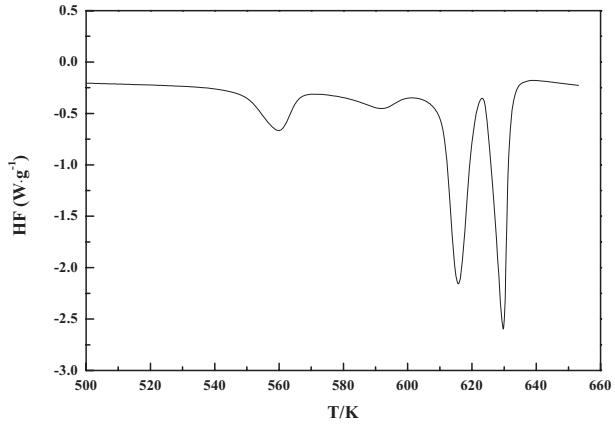

Fig. 2. DSC plot of disodium sebacate.

3. Thermodynamic models

In this paper, the modified Apelblat equation, the λ*h* model and the NRTL model were applied to correlate the solubility of disodium sebacate in the binary solvent mixtures, including (water + methanol), (water + acetone) and (water + DMF). In addition, the dissolution thermodynamic properties of disodium sebacate in different

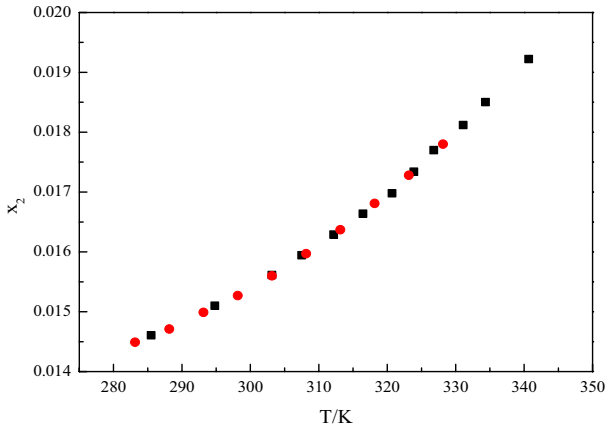

Fig. 3. Comparison of experimental solubility data of disodium sebacate with data from Xia [6]. in water. (● represents experimental data in water which were obtained in this work. ■ represents solubility data in water Xia).