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Determination and correlation of solubility with thermodynamic analysis of lidocaine hydrochloride in pure and binary solvents

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ABSTRACT

The objective of this work was to measure and correlate the solubility of lidocaine hydrochloride in eight pure solvents, including ethanol, n-propanol, isopropanol, n-butanol, isobutanol, acetone, methyl acetate, water, and binary mixtures at (291.15 to 331.15) K by using gravimetric method under atmospheric pressure. The results reveal that the solubility of lidocaine hydrochloride increases with increasing temperature in all solvent selected. The modified Apelblat equation, van't Hoff equation, λh equation, Wilson model and NRTL model were successfully used to correlate the experimental solubility in pure solvents and binary solvent mixtures. In addition, the thermodynamic properties of dissolution of Lidocaine hydrochloride such as Gibbs energy (ΔG°_{sol}), molar enthalpy of dissolution (ΔH°_{sol}), and molar entropy of dissolution (ΔS°_{sol}) were calculated. Consequently, the experimental solubility and correlation equations can be used as essential data and simulation models in the purification and separation of lidocaine hydrochloride.

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1. Introduction

Lidocaine hydrochloride, known as 2-Dimethylamino-N-(2,6-dimethylphenyl)acetamide hydrochloride, is a white crystalline powder. The formula is $C_{14}H_{25}ClN_2O_2$, It is easily soluble in water, ethanol and organic solvents. Lidocaine hydrochloride is recrystallized from Lidocaine and acidified with hydrochloric acid. The molecular structure of lidocaine hydrochloride is presented in Fig. 1. There are many scientific studies on the pharmacological effects of lidocaine hydrochloride, including anesthesia [1] and antiarrhythmic therapy [2]. Most research work was focusing on the pharmacological effects, but no solution dynamics were reported. Therefore, the study of lidocaine hydrochloride solid-liquid equilibrium has a great significance.

As is known to all, the solubility properties of solute is similar to the solubility properties of the solvent composition with maximum solubility. Solubility properties can also help estimate a suitable ratio of solvent for maximum solubility. The solubility of solid compounds in pure and mixed solvents plays an important role in the determination of proper solvents of crystallization processes. Moreover, solubility is an crucial physicochemical parameter in the process of medicine discovery development [3, 4].

In this experiment, the solubilities of lidocaine hydrochloride in ethanol, n-propanol, isopropanol, n-butanol, isobutanol, acetone, methyl acetate, water, and binary mixtures (ethanol + water) from (291.15 to 331.15) K at atmospheric pressure were measured. Moreover, the experimental solubility values in mono solvents and binary mixtures were correlated by the modified Apelblat equation, van't Hoffequation, λhequation, nonrandom two-liquid (NRTL) equation, and Wilson equation. Furthermore, the enthalpy change (ΔH°_{sol}), the entropy change (ΔS°_{sol}), and the Gibbs free energy change (ΔG°_{sol}) in the dissolution process of lidocaine hydrochloride in pure solvents and mixed solvents were calculated. To further understand the dissolving process, the above models play an important role in obtaining a lot of solubility data which can not only conduct us in operation of the crystallization process but also help us to understand the dissolving mechanisms and driving force of the dissolving process of lidocaine hydrochloride.

2. Experimental section

2.1. Materials

The powder of lidocaine hydrochloride was purchased from Beijing HWRK Chem Co., Ltd., with a mass fraction purity higher than 0.99. Ethanol, n-propanol, isopropanol, n-butanol, isobutanol, acetone, water, and methyl acetate were analytical research grade reagents from Beijing Chemical Works of China with the mass fraction purities higher than 0.995. Distilled-deionized water was selected. All of the chemicals were used in this study without further purification. The details of the above materials are listed in Table 1.

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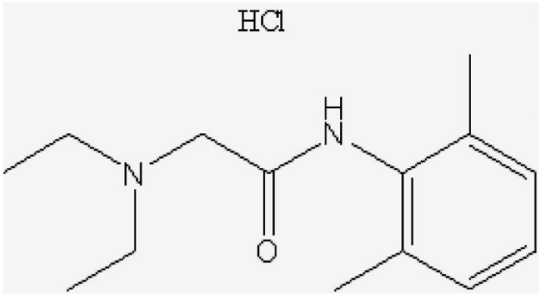

Fig. 1. Chemical structure of lidocaine hydrochloride.

2.2. Apparatus and procedure

The melting temperature T_{melt} of lidocaine hydrochloride were measured for modeling the solid-liquid equilibrium by means of a differential scanning calorimetric instrument (TGA/DSC1/1600LF, Mettler Toledo Co., Switzerland) under protection of nitrogen with a flow rate of 100 ml/min. With the heating rate of 10 K/min, about 5 mg samples were transferred into standard DSC aluminum pans using micropipette and an empty pan was used as reference [5, 6]. The standard uncertainty for Tm is 0.2 K.

The melting point of lidocaine hydrochloride was 80.53 °C. $\Delta_{fus}H$ was 103.04 J/g. The DSC curve is shown as in Fig. 2.

2.3. Measurement of the solubility of lidocaine hydrochloride

In this work, excessive amount of solid lidocaine hydrochloride were added to corresponding solvent mixtures and kept at a certain temperature set up temperature already by a thermostatic water bath shaking table (Shanghai Yi heng Scientific Instrument Co., LTD) with an accuracy of T = ±0.05 K. To reach the solid-liquid equilibrium state, the solutions were shaken for at least 72 h in the bath. Then turning off the shaking and keeping standing for about 12 h to make the undissolved substances to settle down. Subsequently, 5 ml of the supernatant was withdrawn by the syringe filter (0.22 μm) and moved into pre-weighted evaporating dishes. Then the total weight was weighed immediately by the analytical balance. After that, the dishes were transferred into a vacuum oven (Tianjin Taisite Instrument Co., Ltd.., China), weighed until the solvent completely evaporated (over 12 h) and the mass of the solid residue was measured. Each experiment was repeated three times, and the average value was used as the final result.

The mole fraction solubility of lidocaine hydrochloride (x_1) in pure solvents was calculated by Eq. (1) [7].

$$x_1 = \frac{m_1/M_1}{m_1/M_2 + m_2/M_2} \tag{1}$$

where m_1 and m_2 represent the mass of the lidocaine hydrochloride and solvent, M_1 and M_2 are the respective molar mass.

Table 1
The purity and sources of experimental chemicals.

Chemicals	Mass fraction purity	Sources
Lidocaine hydrochloride	99%	Beijing Warwick Rick Co., Ltd
Ethanol	≥99.5%	Beijing Chemical Works, China
n-propanol	≥99.5%	Beijing Chemical Works, China
Isopropanol	≥99.5%	Beijing Chemical Works, China
n-butanol	≥99.5%	Beijing Chemical Works, China
Isobutanol	≥99.5%	Beijing Chemical Works, China
Acetone	≥99.5%	Beijing Chemical Works, China
Methyl acetate	≥99.5%	Beijing Chemical Works, China

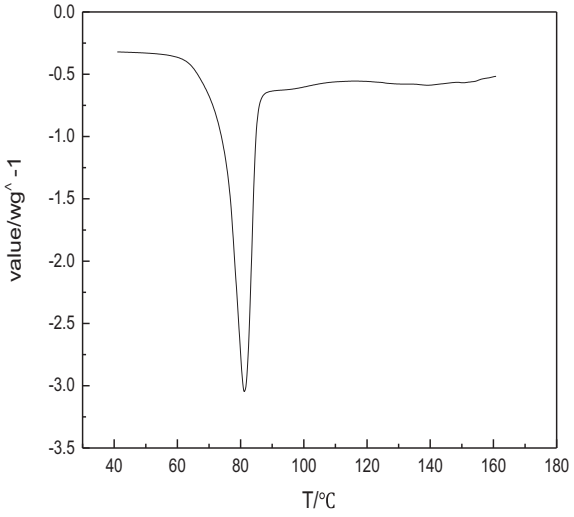

Fig. 2. DSC spectra of lidocaine hydrochloride.

The mass fraction of ethanol (w) in mixed solvent varied from 0.1 to 0.9 in intervals of 0.1; the mass fraction of ethanol in mixed solvents was obtained by Eq. (2).

$$w = \frac{m_3}{m_2 + m_3} \tag{2}$$

where m_2, m_3 represent the mass of water, ethanol respectively.

The mole fraction solubility of lidocaine hydrochloride (x_1) in different ethanol concentration of the mixed solvents at different temperatures is obtained by Eq. (3).

$$x_1 = \frac{m_1/M_1}{m_1/M_1 + m_2/M_2 + m_3/M_3} \tag{3}$$

where m_1, m_2, m_3 represent the mass of lidocaine hydrochloride, water, ethanol; M_1, M_2,and M_3 are the molar mass of lidocaine hydrochloride, water, ethanol, respectively.

3. Results and discussion

3.1. Solubility data of lidocaine

The solubility data of the lidocaine hydrochloride are listed in Tables 2 and 3 in pure and binary solvents, respectively. With the corresponding solubility curves plotted in Figs. 3 and 4. Combining the data in Figs. 3 and 4, it could be found that the solubility of lidocaine hydrochloride increased as the temperature increased. And it is obvious that the maximum solubility is in n-propanol, and the minimum solubility is in acetone. The solubility order in pure solvents is: n-propanol > isobutanol ≈ isopropanol > ethanol > n-butanol > water > methyl acetate > acetone, whose sequence was not consistent with the polar sequence of solvents. It is known to all that the polarity of the solvents might not be the only factor that determines the solubility of different form of lidocaine hydrochloride in the selected solvents. To sum up, a lot of factors that influence solubility of lidocaine hydrochloride include the intermolecular interaction of the solution molecule and the physicochemical properties of solute and solvents, such as the structure, functional group, and so on.

The solubility of lidocaine hydrochloride in mixed solvents increased with the increasing of the mass fraction of ethanol, since the solubility of lidocaine hydrochloride in water much smaller relatively than in ethanol.

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