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Short communication

Thermodynamics of the solubility of lomefloxacin in methanol, ethanol, 1-propanol, 2-propanol, acetone, and chloroform from 293.15 to 323.15 K

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ABSTRACT

The solubilities of lomefloxacin in methanol, ethanol, 1-propanol, 2-propanol, acetone, and chloroform have been determined from 293.15 to 323.15 K by a static equilibrium method. The experimental data were correlated with the modified Apelblat equation. The positive $\Delta_{sol}H$ and $\Delta_{sol}S$ for each system revealed that lomefloxacin being dissolved in each solvent was an entropy-driven process.

1. Introduction

Lomefloxacin is a member of quinolones that are widely used in agriculture to prevent diseases in livestock and to treat illness; therefore, soil and groundwater body have been seriously contaminated. The solubility plays a prominent role in the prediction of the environmental fate of chemicals and can characterize transportation through membranes and the topical activity of drugs [1]. In determining the transport of lomefloxacin in the environment and assessing its risk to terrestrial and aquatic ecosystems, it is necessary to know its solubilities in various solvents. However, only a limited amount of solubility data for lomefloxacin has been reported from 298.15 to 313.15 K [2–5]. In this study, solubilities of lomefloxacin in methanol, ethanol, 1-propanol, 2-propanol, acetone, and chloroform have been measured from 293.15 to 323.15 K. The experimental data were correlated with the modified Apelblat equation [6,7].

2. Experimental methods and apparatus

2.1. Materials

Lomefloxacin obtained from Daming Biotech was further purified by recrystallization from aqueous solutions. After filtration and drying, their purity was determined by UV spectrometry (type UV-2401PC, Shimadzu), to be 0.996 in mass fraction. Methanol, ethanol, 1-propanol, 2-propanol, acetone, and chloroform with mass fraction purities greater than 0.996, 0.998, 0.997, 0.996, 0.997, and 0.998 were all obtained from Tianjin Kermel Chemical Reagent (China) without any further purification.

2.2. Apparatus and procedure

The solubility was measured by a static equilibrium method [8]. Nearly 100 mg of lomefloxacin was added separately to 50 mL of each solvent in glass flasks. The mixtures were then stirred in a mechanical shaker for 1 h. Samples were then allowed to stand in water baths (type 501, Shanghai Laboratory Instrument Works) kept at the appropriate temperature (±0.02 K). The equilibrium of other quinolones has been reported to be achieved after 30 h. Therefore, in this work, the initial equilibrium time of the saturated solution was 72 h; then, it was analyzed once every 5 h until the analyzing results were replicated three consecutive times. After this time, the supernatant solutions were filtered to ensure that they were free of particulate matter before sampling. We determined concentrations by measuring UV absorbances after appropriate dilution and interpolation from previously constructed calibration curves for each system. To permit conversion between molarity and mole-fraction concentration scales, the density of the saturated solutions was determined with a digital density meter. All of the solubility experiments were repeated at least three times, and the mean values were considered to be the measured results. The uncertainty of temperature measurements was ±0.05 K. The reproducibility of temperature measurements was 0.1 K, which

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Table 1
Mole fractions solubilities (x) of norfloxacin in water compared with literature data at 298.15 K.

System	$10^5 x_{exptl}$	$10^5 x_{ref}$	100RD
Norfloxacin + water	2.270 [5]	2.258 [3]	0.53

corresponds to a relative deviation in composition smaller than 2.0%. The results showed that the deviation of the measured solubility from the literature values [3] was less than 1.0%. Therefore, the reliability of the experimental apparatus was verified.

3. Results and discussion

The solubilities of norfloxacin in water listed in Table 1 are measured to complete the data reported in literature [3].

The temperature dependence of lomefloxacin solubility in methanol, ethanol, 1-propanol, 2-propanol, acetone, and chloroform has been described by the modified Apelblat equation [6,7]

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

where x is the mole fraction of lomefloxacin, T is the absolute temperature, and A, B, and C are parameters determined by least square analysis. The values of these parameters are listed in Table 3. The relative deviations (RD values) between the experimental and calculated values of solubilities are also calculated by Eq. (2) and are listed in Table 2.

$$\mathrm{RD} = \left(\frac{x - x_c}{x}\right) \quad (2)$$

Table 2
Solubility data of lomefloxacin in different solvents and the regression results obtained using the modified Apelblat equation.

T (K)	$10^5 x$	100RD	T (K)	$10^5 x$	100RD
Lomefloxacin + methanol					
293.15	3.867	−0.29	313.15	10.52	−0.012
298.15	4.757	0.58	318.15	14.48	−0.78
303.15	5.949	−0.46	323.15	20.89	0.46
308.15	7.848	0.51			
Lomefloxacin + ethanol					
293.15	1.222	0.30	313.15	3.735	0.58
298.15	1.639	−0.78	318.15	4.705	−0.19
303.15	2.217	0.76	323.15	5.898	−0.029
308.15	2.863	−0.63			
Lomefloxacin + 1-propanol					
293.15	1.069	0.25	313.15	3.036	0.27
298.15	1.364	−0.21	318.15	3.989	−0.40
303.15	1.756	−0.66	323.15	5.334	0.055
308.15	2.321	0.70			
Lomefloxacin + 2-propanol					
293.15	0.5738	−0.20	313.15	2.232	−0.52
298.15	0.8552	0.14	318.15	2.926	1.0
303.15	1.231	0.83	323.15	3.616	−0.34
308.15	1.668	−0.91			
Lomefloxacin + acetone					
293.15	0.8633	0.078	313.15	2.566	−0.33
298.15	1.099	−0.12	318.15	3.535	−0.16
303.15	1.429	−0.29	323.15	4.952	0.12
308.15	1.917	0.71			
Lomefloxacin + chloroform					
293.15	4.079	−0.035	313.15	19.63	−0.18
298.15	5.939	0.46	318.15	30.35	0.72
303.15	8.634	−0.77	323.15	46.52	−0.40
308.15	13.02	0.21			

Note: The experimental uncertainties on T and x are estimated to be ±0.05 K and 2.4×10^{-8}, respectively.

Table 3
Parameters in the modified Apelblat equation for different systems.

System	A	B	C	100ARD
Lomefloxacin + methanol	−1018.6	41,623	152.52	0.44
Lomefloxacin + ethanol	196.85	−13,720	−28.405	0.47
Lomefloxacin + 1-propanol	−409.14	13,891	61.666	0.36
Lomefloxacin + 2-propanol	622.86	−33,935	−91.392	0.57
Lomefloxacin + acetone	−698.23	26,731	104.81	0.26
Lomefloxacin + chloroform	−664.96	23,439	101.20	0.39

The average relative deviations (ARD values) for each system in this study are also calculated by Eq. (3) and are given in Table 3.

$$\mathrm{ARD} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{x_i - x_{ci}}{x_i}\right| \quad (3)$$

The data in Tables 2 and 3 indicate that the calculated solubilities show good agreement with the experimental data, which demonstrates that the modified Apelblat equation can be used to correlate the solubility data of lomefloxacin in different solvents. The relative deviations among the 42 data points for the studied systems do not exceed 1.0%, and the total average relative deviation is 0.41%.

By using the data shown in Table 2, we plotted the solubility curves for the studied systems in Fig. 1. It is evident that the solubility of each system is low. The solubility data of lomefloxacin in methanol, ethanol, 1-propanol, 2-propanol, acetone, and chloroform showed a flat uptrend when the temperature increased. Moreover, the structure of lomefloxacin indicates that the molecule is highly aromatic and the functional groups may not contribute much to the aqueous solubility. So, the solubility is minimum in 2-propanol and maximum in chloroform.

According to a pseudochemical reaction process [9], the dissolution process of solid, S, in liquid, W, can be expressed as S + W = SW; the relationship of its dissolution equilibrium constants and activities can be expressed as

$$K_i = \frac{a_i}{a_S a_W} \quad (4)$$

where a_i is the activity of lomefloxacin in solution, a_S and a_W are the activities of pure solid, S, and pure liquid, W, respectively.

Because of S and W all in standard states, it is believed that each of a_S and a_W is considered to be a constant.

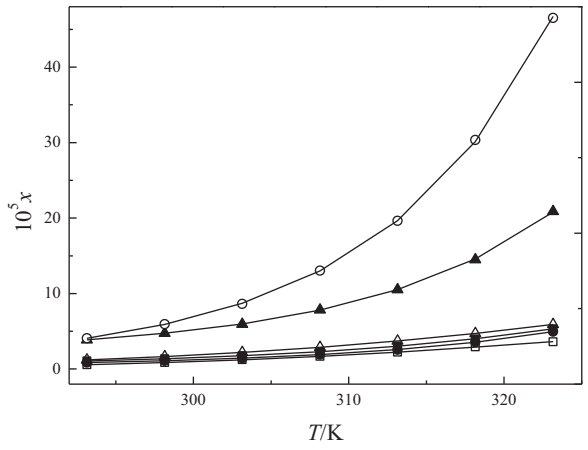

Fig. 1. Solubilities of lomefloxacin in studied solvents: ▲, lomefloxacin + methanol; △, lomefloxacin + ethanol; ■, lomefloxacin + 1-propanol; □, lomefloxacin + 2-propanol; •, lomefloxacin + acetone; ○, lomefloxacin + chloroform; —, calculated from Eq. (1).