Solubility of Sucralose in Different Solvents from (283.15 to 333.15) K

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The solubility of sucralose in water, methanol, ethanol, and isopropyl alcohol from (283.15 to 333.15) K was measured by an isothermal method. The results show that the solubility of sucralose in the four solvents increases with the increasing temperature. The experimental solubility data were correlated by the modified Apelblat equation, and the calculated values were in good agreement with the experimental data.

Introduction

Sucralose (1,6-dichloro-1,6-dideoxy-β-D-fructofuranosyl-4-chloro-4-deoxy-α-D-galactopyranoside, CAS Registry No. 56036-13-2, molecular mass: 397.6335) is a new high-quality intense sweetener discovered by Hough and his colleagues,[1,2] which was approximately 600 times sweeter than sucrose without an unpleasant aftertaste. It was one of a series of chlorodeoxy derivatives of sucrose synthesized by selective chlorination of sucrose at three of the primary hydroxyl groups.[2,3] The crystal and molecular structure of sucralose was determined by Kanters et al.[4] The chemical structure of sucralose is shown in Figure 1. Compared with other sweeteners, sucralose has the advantage of high stability at elevated temperature and low pH. Sucralose is noncaloric and noncariogenic and has no effect on blood glucose. Therefore, sucralose is widely used in food and beverages, especially ideal for people with diabetes or obesity.[5,6]

In industrial production, sucralose was often refined from solution by cooling crystallization to obtain high purity and quality. The investigation of the solubility of sucralose in different solvents is very important for choosing the proper solvent and optimizing the crystallization process. The solubility of sucralose in water over the temperature range from (293.15 to 333.15) K has been measured before.[7] However, the solubility data in organic solvents have not been studied until now.

In the present work, the solubility of sucralose in water, methanol, ethanol, and isopropyl alcohol from (283.15 to 333.15) K was experimentally measured by an isothermal method. The data obtained in this work were compared with those reported in literature.

Experimental Section

Materials. Sucralose (purity > 99.8 %) was supplied by Techno Food Ingredients Co., Ltd. Methanol, ethanol, and isopropyl alcohol used for the experiments were of analytical reagent grade, and the mass fractions were 99.5 %, 99.7 %, and 99.7 %, respectively. Deionized water was used throughout the experiments.

Sample Preparation. The solubility was measured by the isothermal method.[8,9] An excess amount of sucralose was added to a certain mass of solvent in a jacked glass vessel maintained at a desired temperature with continuous stirring. The temperature was controlled by circulating water through the outer jacket from a thermostatically controlled super constant temperature water bath (type DC-2030, Shanghai Sunny Hengping Scientific Instrument Co., Ltd.) with an accuracy of 0.05 K. After stirring for at least 4 h, the suspended solution was kept still for 1 h. Then, the supernatant liquid was filtered, and the filtrate was diluted by a certain fold for high performance liquid chromatography (HPLC) analysis. Each measurement was repeated three times, and the uncertainty of the mole fraction solubility values is established to be within 0.5 %.

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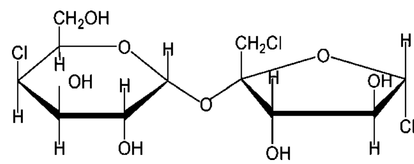

Figure 1. Structure of sucralose.

Table 1. Mole Fraction Solubility of Sucralose in Water, Methanol, Ethanol, and Isopropyl Alcohol from (283.15 to 333.15) K

T/K	$10^3\ x_1$	$10^2[(x_1 - x_1^{cal})/x_1]$	T/K	$10^3\ x_1$	$10^2[(x_1 - x_1^{cal})/x_1]$
		Water			
283.15	10.69	0.315	313.15	19.54	−3.54
288.15	11.54	0.199	318.15	22.30	−1.89
293.15	12.31	−3.10	323.15	25.90	1.81
298.15	14.63	3.12	328.15	28.49	0.552
303.15	16.42	2.91	333.15	31.43	0.00794
308.15	18.24	1.55			
		Methanol			
283.15	30.74	−1.53	313.15	41.47	0.0570
288.15	31.54	0.427	318.15	44.90	−0.225
293.15	32.81	1.67	323.15	48.53	−0.971
298.15	34.31	1.67	328.15	52.38	−1.94
303.15	36.15	1.02	333.15	59.60	2.36
308.15	38.33	−0.0954			
		Ethanol			
283.15	8.431	0.129	313.15	20.17	−0.338
288.15	9.764	−1.58	318.15	22.79	0.0256
293.15	12.00	3.15	323.15	24.84	−2.52
298.15	14.33	5.65	328.15	28.08	−0.657
303.15	15.83	1.46	333.15	32.21	3.21
308.15	18.41	3.05			
		Isopropyl Alcohol			
283.15	3.609	1.53	313.15	8.536	−5.56
288.15	3.894	2.61	318.15	11.02	2.53
293.15	4.401	1.73	323.15	12.76	0.723
298.15	5.334	3.82	328.15	14.97	1.38
303.15	6.236	0.726	333.15	17.08	0.236
308.15	7.886	5.03			

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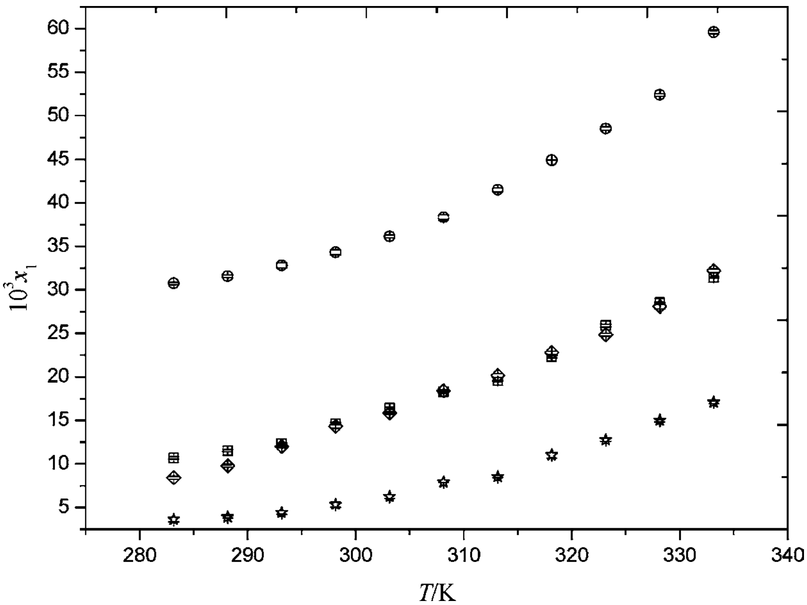

Figure 2. Mole fraction solubility of sucralose at different temperatures in four pure solvents: □, water; ○, methanol; ◇, ethanol; ☆, isopropyl alcohol.

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

solvent	A	B	C	10^3 rmsd
water	−7.8705	326.43	1.1917	0.377
methanol	−14.970	641.21	2.2559	0.622
ethanol	−5.7195	225.11	0.87370	0.494
isopropyl alcohol	−6.7619	287.09	1.0187	0.229

Sample Analysis. The amount of sucralose in each solvent was determined by the HPLC system (Agilent 1100) using a refractive index detection (Agilent G1362A) and a Sepax HP-C18 column (4.6 × 250 mm, 5 μm). The mobile phase was acetonitrile (1) + methanol (2) + water (3) with a volume fraction ratio of 15:5:80. The flow rate of the mobile phase was 1.0 mL·min $^{-1}$. The analysis was performed at 323.15 K.

The mole fraction solubility (x_1) of sucralose in different solvents could be obtained from eq 1

$$x_1 = \frac{m_1/M_1}{m_1/M_1 + m_2/M_2} \qquad (1)$$

where m_1 and m_2 represent the masses of solute and solvent, respectively, and M_1 and M_2 are the molecular weight of the solute and solvent.

Results and Discussion

The measured solubilities of sucralose in water, methanol, ethanol, and isopropyl alcohol from (283.15 to 333.15) K are listed in Table 1 and more visually plotted in Figure 2, and the standard deviations of the experimental data are represented by an error bar. Compared with the solubility data in water reported in the literature, the data in this work were 5 % higher. It can be seen that the solubility of sucralose in all of the four solvents increases with the increasing temperature. It should be noted that the solubility of sucralose is especially higher in methanol but much lower in isopropyl alcohol. The temperature dependence of the solubility of sucralose in the pure solvents can be correlated by the modified Apelblat eq 2[9−11]

$$x_1 = A + \frac{B}{T/\mathrm{K}} + C \ln(T/\mathrm{K}) \qquad (2)$$

where x_1 is the mole fraction solubility in different solvents and T is the absolute temperature. A, B, and C were obtained by fitting the experimental solubility data and are presented in Table 2 together with the corresponding root-mean-square deviations (rmsd's). The rmsd is defined as

$$\mathrm{rmsd} = \sqrt{\frac{\sum_{i=1}^{N} (x_1 - x_1^{\mathrm{cal}})^2}{N}} \qquad (3)$$

where N is the number of experimental points and x_1 and x_1^{cal} represent the mole fraction solubility of the experiment and that calculated from eq 2, respectively.

From Table 2, it is seen that the calculated solubility by the modified Apelblat equation was in good agreement with the experimental values.

Conclusions

(1) The solubility of sucralose in water, methanol, ethanol, and isopropyl alcohol is a function of temperature and increases with an increase of temperature.

(2) Methanol, water, and ethanol all present good ability of dissolving sucralose, and the mole fraction solubility of sucralose in methanol is much higher than in the other three solvents. In view of low toxicity and low price, water can be the most suitable solvent for purification and crystallization.

(3) The calculated solubility data of sucralose are in good agreement with the experimental values. The experimental solubility data and correlation equation in this work might be significant for the purification and crystallization of sucralose in industry.

Note Added after ASAP Publication: This paper was published ASAP on January 14, 2010. Equation 2 was updated. The revised paper was reposted on June 4, 2010.

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