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Short Communication

Thermodynamic of *β*-cyclodextrin in sucrose solution

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ABSTRACT

Based on the solubility of β-cyclodextrin in 5% sucrose solution, the dissolution enthalpy and dissolution entropy have been calculated from the experimental data. The mutual interaction between solvent and solute has been discussed briefly.

Keywords: Solubility, β-cyclodextrin, dissolution enthalpy, dissolution entropy.

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INTRODUCTION

Cyclodextrins are polysaccharides mainly composed of six to eight D-glucose monomers linked by α-(1,4)-glycosidic bonds, which assume a truncated-cone shape with the primary hydroxyl groups on the narrow side and the secondary hydroxyl groups on the wider side (Liu et al., 2017). This structure possesses a hydrophobic inner cavity and a hydrophilic outer surface. The cavity is a necessary prerequisite for cyclodextrins to spontaneously incorporate guest molecules. β-cyclodextrin is a common one which is obtained by seven D-glucopyranose polymerization, it is an important food and pharmaceutical additive. But the solubility of β-cyclodextrin in water is less, which restrict its applications. In order to improve its solubility, sucrose was introduced into cyclodextrin molecules. The studies on the intersolubility of β-cyclodextrin and sucrose is important, there is little report on the solubility of β-cyclodextrin in sucrose solution, therefore in this study, the solubility of β-cyclodextrin in 5% sucrose solution have been determined. Moreover, there are little essays which explain dissolution enthalpy and dissolution entropy of β-cyclodextrin in sucrose solution. Therefore, we calculated the data of dissolution enthalpy and dissolution entropy for β-cyclodextrin dissolving in sucrose, also, the reason for the dissolving phenomenon has been explained in brief.

EXPERIMENTAL

Materials

β-cyclodextrin is of AR grade, and was obtained from Shanghai Chemical Reagent Co. Sucrose was of AR grade, which was obtained from Sinopharm Chemical Reagent Co. Deionized water was used.

Solubility measurement

The solubility of β-cyclodextrin in 5% sucrose solution had been measured by a laser monitoring technique from 293.45 to 357.45 K at atmospheric pressure, and the experimental process as same as stated in Li et al. (2009). The solubility expressed by mole fraction was calculated as follows:

$$x = \frac{m_1/M_1}{m_1/M_1+m_2/M_2+m_3/M_3} \quad (1)$$

Where m_1 represents the mass of solute, m_2 and m_3 represent the mass of solute and solvent respectively in the sucrose solution. M_1, M_2 and M_3 are the molecular masses, respectively.

Test of apparatus

To prove the feasibility and the uncertainty of the measurement, the solubility of NaCl in water was measured and compared with the values reported in the literature (Li et al., 2014). The experimental measurements agreed with the reported values with a mean relative deviation of 1.24%. The measured values are listed in Table 1.

Table 1. Solubility of NaCl in water.

T/K	x	x (lit)[3]	100RD
293.15	0.1015	0.0999	1.58
313.15	0.1021	0.1011	0.98
333.15	0.1045	0.1033	1.15
373.15	0.1108	0.1094	1.26

RESULTS AND DISCUSSION

The measured solubilities of β-cyclodextrin in 5% sucrose solution at different temperatures were presented in Table 2. The experimental data were correlated with the modified Apelblat equation:

$$\ln x = A + \frac{B}{T} + C\ln T \quad (2)$$

Where *x* is the mole fraction solubility of β-cyclodextrin. *T* is the absolute temperature. *A*, *B* and *C* are the model parameters.

Fit quality of Apelblat equation was evaluated by Root Mean Square Deviation (RMSD), Relative Deviation (RD), Relative Average Deviation (RAD) and the equation of RMSD, RD and RAD can be seen in Li et al. (2009), the values are listed in Table 3. From Table 3, it can be found that the calculated solubilities show good agreement with the experimental data.

Thermodynamic functions related with solubility are mainly dissolution enthalpy and dissolution entropy, namely *ΔH* and *ΔS*, which can be obtained through a series of thermodynamic equations. The dissolution process of solid S in liquid W can be expressed as S+W=SW according to a pseudochemical reaction process (Wang, 2001), the relationship between its dissolution equilibrium and activities can be expressed as:

$$K_i = \frac{a_i}{a_s \times a_w} \quad (3)$$

Where a_i stands for the activity of β-cyclodextrin in the solution, a_s and a_w represent the activities of pure solid S and pure liquid W respectively. Due to the standard states of S and W, a_s and a_w are believed to be constants. The relationship between the activity a_i and the mole fraction x_i can be shown as below:

$$a_i = \gamma_i \times x_i \quad (4)$$

Therefore Equation 3 can be written as:

$$K_i = \frac{\gamma_i \times x_i}{a_s \times a_w} \quad (5)$$

Where γ_i is the activity coefficient of β-Cyclodextrin, and x_i is the mole fraction of β-cyclodextrin in 5% sucrose solution.

Table 2. Mole fraction solubilities of β-cyclodextrin in sucrose solution.

T	$x^i \times 10^4$	$x^{ci} \times 10^4$	RD
293.45	2.5254	2.0534	0.1869
298.55	3.1629	2.7116	0.1427
303.35	3.9798	3.5106	0.1179
308.25	4.8223	4.5541	0.0556
312.65	5.7222	5.7369	-0.0026
318.25	7.2819	7.6676	-0.0530
323.25	9.6630	9.8998	-0.0245
328.15	12.1283	12.6772	-0.0453
333.05	15.1430	16.1850	-0.0688
337.55	19.6502	20.2032	-0.0281
342.95	25.8855	26.2783	-0.0152
347.55	32.7985	32.7862	0.0004
352.65	42.4532	41.7832	0.0158
357.45	52.8033	52.3556	0.0085

By logarithmic treatment, equation (5) can be changed into:

$$\ln K_i = \ln x_i + J \quad (6)$$

Where J = $\ln\gamma_i - \ln(a_s * a_w)$, which is a constant independent off temperature.

Based on Gibbs equation and the modified Van't Hoff method (Wang et al., 2014), the equation for calculating molar enthalpies of dissolution ΔH can be obtained as follows:

$$\Delta H = -R \times \frac{d\ln K_i}{dT^{-1}} \quad (7)$$

That is to say,

$$\Delta H = -R \times \frac{d\ln x_i}{dT^{-1}} \quad (8)$$

Then Equation 2 is used to obtain the derivation and substitute it into Equation 8, thus Equation 9 is given below:

$$\Delta H = R \times T \times (C - \frac{B}{T}) \quad (9)$$

According to the thermodynamic equation between enthalpy and entropy (Prausnitz et al., 1999), the dissolution ΔS can be obtained as below:

$$\Delta S = R \times (C - \frac{B}{T}) \quad (10)$$

According to the parameters of modified Apelblat equation listed in Table 3, Δ*H* and Δ*S* can be calculated by Equations 9 and 10, which is listed in Table 4.

Table 3. Parameters of β-cyclodextrin in sucrose solution.

A	B	C	R^2	RMSD × 10^5	RAD
-122.21	974.79	19.43	0.9988	1.32	0.055

Table 4. *ΔH* and *ΔS* of β-cyclodextrin in 5% sucrose solution.

T (K)	*ΔH* (KJ·mol^{-1})	*ΔS* (J·mol^{-1}·K^{-1})
293.45	39.299	133.92
298.55	40.123	134.39
303.35	40.899	134.82
308.25	41.690	135.25
312.65	42.401	135.62
318.25	43.306	136.07
323.25	44.113	136.47
328.15	44.905	136.84
333.05	45.696	137.20
337.55	46.423	137.53
342.95	47.296	137.91
347.55	48.039	138.22
352.65	48.863	138.56
357.45	49.638	138.86

From Table 4, it can be found that dissolution enthalpies *ΔH* and dissolution entropies ΔS of β-cyclodextrin in 5% sucrose solution are positive and they increase with the increase of temperature. The positive Δ*S* for the process indicate the dissolving process is entropy-driven. For the reason is that entropy is a measurement of chaos for the system, the sucrose solution is quite in order, while if added the solute into the orderly solvent will raises the chaos degree of the system, and increase the dissolving entropies. The positive *ΔH* shows the process is endothermic which goes against the dissolving process, the reason might be that there exists strong interactions between solute and solution, in order to dissolve β-cyclodextrin in sucrose solution, it is essential to absorb enough heat to destroy the force between the molecules, therefore, the process of β-cyclodextrin dissolution in sucrose solution is endothermic.

CONCLUSION

The solubilities of β-cyclodextrin in sucrose solution were measured, and the experimental data were correlated with the Apelblat equation, also the dissolution enthalpies *ΔH* and dissolution entropies *ΔS* were estimated. The positive *ΔH* and *ΔS* reveal the process is endothermic and entropy-driven. The experimental solubility and the calculated dissolution enthalpies *ΔH* and dissolution entropies *ΔS* can provide some essential data for the application of β-cyclodextrin.

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