

Measurement and correlation of solubility of xylitol in binary water+ethanol solvent mixtures between 278.00 K and 323.00 K

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Abstract—The solubility of xylitol in ethanol+water solvent mixtures was measured at temperatures ranging from 278.00 K to 323.00 K at atmospheric pressure by using a laser technique. The results of these measurements were correlated by the combined nearly ideal binary solvent CNIBS/Redlich-Kister equation. The experimental solubility and correlation equation in this work can be used as essential data and models in the purification process of xylitol. The variant 2 in the CNIBS/R-K models was confirmed to be more adaptable to predict solubility of xylitol in binary ethanol+water system. Using the experimentally measured solubilities, the thermodynamic properties of dissolution of xylitol, such as Gibbs energy, molar enthalpy of dissolution, and molar entropy of dissolution, were calculated.

Key words: Xylitol, Solubility, Measurement, Correlation, Thermodynamic Properties

INTRODUCTION

Xylitol, a pentitol with high sweetening power and anticariogenic properties, is one kind of sugar substitute in food production, perfumery, pharmaceuticals, and chemistry. Xylitol crystals are white, odorless, and hygroscopic, having a negative heat of solution, a melting point between 365.00 K and 369.00 K, exhibiting various solubility in different kinds of solvents [1-4].

In industrial manufacture, xylitol is purified through crystallization from solution as the final step and dilution crystallization generally is preferable. It is well known that crystallization is the key step, since, in many respects, it determines the yield and quality of the target product. Therefore, crystallization processes are the critical steps that determine the quality of final product, and knowing the solubility of the product is a necessary condition in order to design the crystallization process properly. What's more, to determine proper solvents and to design an optimized production process, it is necessary to know the solubility of the target product in different solvent systems. Because xylitol in pure ethanol is slightly soluble and is extremely soluble, water+ethanol can be an ideal system for the dilution crystallization of xylitol. However, from a review of the literature, it was found that no experimental solubility data in binary ethanol+water solvent mixtures was available. In this paper, the solubility of xylitol in binary ethanol+water solvent mixtures was experimentally determined at the temperatures ranging from 278.00 K to 323.00 K and at atmospheric pressure using a laser technique. The method employed in this work is much faster and more readily credible than the analytical method, which is classified as a synthetic method [5]. Solubility data of xylitol determined can be used to make a further analysis of theoretical yield, control of crystallization process and so on in real industrial crystallization.

Modeling of experimental solubility data enables researchers to represent mathematical aspects of solubility. A number of methods

have been presented to estimate the solubility of solute in solvent mixtures. According to these methods, the solubility of a solute can be predicted in systems. In this work, experimental data were correlated by CNIBS/Redlich-Kister equation. The deviation calculated of the different CNIBS/R-K models was analyzed to enhance the reliability of prediction of these models.

EXPERIMENTAL SECTION

1. Chemicals

The xylitol used for the solubility measurement was purchased commercially from Tianjin Silicon Valley Technology Development Co. Ltd., China, and it was obtained by recrystallizing commercial xylitol obtained. Ethanol used for experiments was analytical grade without further treatment. Distilled deionized water of HPLC grade was used.

2. Apparatus and Procedure

The solubility of xylitol was measured by the last crystal disappearance method. That is, the dissolution of the solute was examined by the laser beam penetrating the vessel. In this experiment, a 100 mL jacked vessel was used to determine the solubility; the temperature was controlled to be constant through a thermostat water bath. The masses of the samples and solvents were weighted using an analytical balance with an uncertainty of ± 0.0001 g.

The solubility of xylitol was determined by using a laser technique [6-9]. During experiments, the fluid in the glass vessel was monitored by a laser beam. Predetermined excess amounts of solvent and xylitol were placed in the inner chamber of the vessel. The content of the vessel was stirred continuously at a required temperature. In the early stage of the experiment, the laser beam was blocked by the undissolved particles of xylitol in the solution, so the intensity of laser beam penetrating the vessel was lower. Along with the dissolution of the particles of the solute, the intensity of the laser beam increased gradually. When the solute dissolved completely, the solution became clear and transparent and the laser intensity reached maximum. Then additional solute of known mass (about 1 to 5 mg)

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was added into the vessel. We repeated this procedure unless the penetrated laser intensity could not return maximum, and at this moment, the last addition of solute could no longer dissolve completely. The interval of addition was 30 min. The total amount of the solute consumed was recorded.

All the experiments were conducted three times, and the mean values were used to calculate the mole fraction solubility. The uncertainty of the experimental solubility values was not more than 0.5%. The saturated mole fraction solubility of the solute (x_A) in solution was obtained as follows:

$$x_A = \frac{m_A/M_A}{m_A/M_A + m_B/M_B + m_C/M_C} \quad (1)$$

In which m_A , m_B and m_C represented the masses of solute, water, and ethanol. M_A , M_B , and M_C are the molecule weight of solute, ethanol, and water, respectively.

RESULTS AND DISCUSSION

1. Solubility Data

To verify the reliability of the method of solubility measurement used, the solubility data of xylitol in pure ethanol and water was compared with the literature. Fig. 1 is the plot of solubility of xylitol in pure ethanol and pure water between 278.00 K and 323.00 K. From Fig. 1, it can be seen that xylitol is extremely soluble in pure water and sharply rises with increase of temperature, while it is slightly soluble in pure ethanol. The solubility data measured in pure ethanol and water are in good agreement with the literature reported [10].

The solubility data of xylitol in ethanol+water binary mixtures

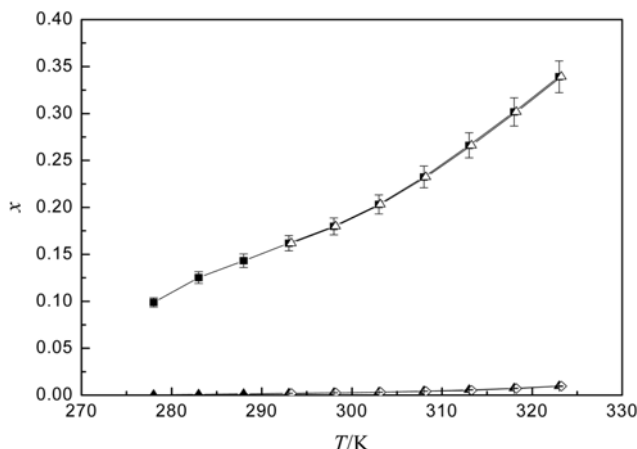


Fig. 1. ■, Solubility plot of xylitol in pure water from 278.00 K to 323.00 K; ▲, Solubility plot of xylitol in pure ethanol from 278.00 K to 323.00 K; △, Solubility plot of xylitol in pure water in literature [15]; ◇, Solubility plot of xylitol in pure ethanol in literature [15].

from 278.00 K to 323.00 K are listed in Table 1. x_c^0 denotes ethanol mole fraction of the binary solvent where solute was not present. From Table 1, it can be seen that solubility of xylitol increases with increasing temperature. At a certain constant temperature, the solubility of xylitol in ethanol+water binary mixtures increases with increasing water content.

2. Data Correlation

The solubility data in Table 1 can be exactly described by the combined nearly ideal binary solvent (CNIBS)/Redlich-Kister mod-

Table 1. Experimental solubility (x_A) of xylitol in binary ethanol (C)+water (B) solvent mixtures at the temperature range from 278.00 K to 323.00 K

x_c^0	$x_A^{exp} 10^3$	$x_A^{cal.1} 10^3$	$x_A^{cal.2} 10^3$	$x_A^{cal.3} 10^3$	x_c^0	$x_A^{exp} 10^3$	$x_A^{cal.1} 10^3$	$x_A^{cal.2} 10^3$	$x_A^{cal.3} 10^3$
T=278.00 K					T=283.00 K				
0.0000	98.30	97.88	98.70	98.70	0.0000	128.8	128.6	125.2	125.2
0.0706	71.20	72.70	72.90	72.90	0.0706	89.70	90.26	90.13	90.13
0.1741	55.20	53.22	53.05	53.05	0.1741	65.00	64.86	65.11	65.11
0.2821	38.30	38.49	38.41	38.41	0.2821	50.40	48.60	48.48	48.48
0.3654	25.90	27.79	27.88	27.88	0.3654	34.40	36.82	36.69	36.69
0.4777	16.90	15.35	15.48	15.48	0.4777	22.60	21.85	21.95	21.95
0.6101	5.700	6.190	6.120	6.120	0.6101	9.700	9.410	9.530	9.530
0.7000	3.400	3.160	2.970	2.970	0.7000	4.700	4.890	4.860	4.860
0.7827	2.600	1.790	1.530	1.530	0.7827	3.600	2.740	2.560	2.560
1.000	0.5000	1.090	0.5100	0.5100	1.000	0.8000	1.400	0.7500	0.7500
T=288.00 K					T=293.00 K				
0.0000	143.9	143.8	143.2	143.2	0.0000	162.5	162.2	161.9	161.9
0.0706	104.9	105.1	105.2	105.2	0.0706	121.5	122.4	122.6	122.6
0.1741	78.70	79.41	79.40	79.40	0.1741	97.00	96.72	96.68	96.68
0.2821	64.70	62.12	62.01	62.01	0.2821	80.10	78.28	78.14	78.14
0.3654	46.20	48.43	48.42	48.42	0.3654	60.00	61.90	61.90	61.90
0.4777	29.70	29.72	29.87	29.87	0.4777	38.20	38.11	38.29	38.29
0.6101	13.70	13.26	13.29	13.29	0.6101	16.20	16.81	16.83	16.83
0.7000	7.200	7.050	6.910	6.910	0.7000	10.10	8.870	8.700	8.700
0.7827	5.000	4.010	3.750	3.750	0.7827	6.700	5.080	4.760	4.760
1.000	1.400	2.130	1.390	1.390	1.000	2.100	3.130	2.100	2.100

Table 1. Continued

x_c^0	$x_A^{exp} 10^3$	$x_A^{cal.1} 10^3$	$x_A^{cal.2} 10^3$	$x_A^{cal.3} 10^3$	x_c^0	$x_A^{exp} 10^3$	$x_A^{cal.1} 10^3$	$x_A^{cal.2} 10^3$	$x_A^{cal.3} 10^3$
T=298.00 K					T=303.00 K				
0.0000	180.6	180.6	179.7	179.7	0.0000	204.2	204.9	203.1	203.1
0.0706	138.0	137.5	137.6	137.6	0.0706	172.9	170.4	170.1	170.1
0.1741	108.5	110.9	110.9	110.9	0.1741	136.8	141.1	141.3	141.3
0.2821	97.20	92.88	92.72	92.72	0.2821	119.8	115.4	115.5	115.5
0.3654	73.60	76.06	76.01	76.01	0.3654	90.90	93.15	93.05	93.05
0.4777	48.50	49.42	49.61	49.61	0.4777	61.70	61.36	61.24	61.24
0.6101	24.00	23.10	23.18	23.18	0.6101	31.00	30.62	30.65	30.65
0.7000	12.40	12.47	12.31	12.31	0.7000	15.90	17.30	17.41	17.41
0.7827	8.800	7.110	6.760	6.760	0.7827	11.00	9.930	10.07	10.07
1.000	2.500	3.550	2.490	2.490	1.000	3.100	3.030	3.130	3.130
T=308.00 K					T=313.00 K				
0.0000	234.4	234.4	232.4	232.4	0.0000	265.5	264.9	266.1	266.1
0.0706	198.7	198.4	198.2	198.2	0.0706	226.2	228.2	228.4	228.4
0.1741	167.8	169.4	169.7	169.7	0.1741	202.3	199.9	199.7	199.7
0.2821	145.9	142.7	142.6	142.6	0.2821	173.2	172.9	172.9	172.9
0.3654	114.8	117.0	116.9	116.9	0.3654	141.8	145.0	145.0	145.0
0.4777	77.60	78.07	78.11	78.11	0.4777	101.8	99.58	99.64	99.64
0.6101	40.90	39.28	39.40	39.40	0.6101	53.40	51.48	51.44	51.44
0.7000	20.70	22.44	22.43	22.43	0.7000	25.10	29.62	29.56	29.56
0.7827	14.70	13.17	13.01	13.01	0.7827	19.40	17.27	17.23	17.23
1.000	4.200	4.860	4.230	4.230	1.000	5.700	5.620	5.670	5.670
T=318.00 K					T=323.00 K				
0.0000	302.2	300.8	301.7	301.7	0.0000	329.1	328.3	339.1	339.1
0.0706	255.7	260.6	260.5	260.5	0.0706	289.1	292.0	293.7	293.7
0.1741	239.0	232.1	232.0	232.0	0.1741	271.7	267.5	266.1	266.1
0.2821	203.6	206.1	206.2	206.2	0.2821	243.7	243.6	243.2	243.2
0.3654	172.3	176.7	176.8	176.8	0.3654	206.7	213.2	213.8	213.8
0.4777	129.5	125.0	124.8	124.8	0.4777	161.6	155.7	156.2	156.2
0.6101	69.10	66.11	65.97	65.97	0.6101	88.90	86.00	85.60	85.60
0.7000	30.30	38.15	38.27	38.27	0.7000	41.90	50.99	50.56	50.56
0.7827	25.00	22.01	22.38	22.38	0.7827	33.60	29.93	29.89	29.89
1.000	7.300	6.380	7.280	7.280	1.000	9.700	8.350	9.680	9.680

x_c^0 is the mole fraction of ethanol in a mixed solvent. x_A^{exp} denotes the experimental solubility data, $x_A^{cal.1}$, $x_A^{cal.2}$ and $x_A^{cal.3}$ denote back-calculated solubility data by variant 1, 2, and 3 of CNIBS/R-K model, respectively

els. Acree and co-workers [10-12] suggested the CNIBS-Kister model.

$$\ln x_A = x_B^0 \ln(x_A)_B + x_C^0 \ln(x_A)_C + x_B^0 x_C^0 \sum_{i=1}^N S_i (x_B^0 - x_C^0)^i \quad (2)$$

As a reasonable mathematical representation, the CNIBS-Kister model can accurately describe how the experimental isothermal solubility of a crystalline solute dissolved in binary solvent mixtures varies with binary solvent composition altering. Moreover, in the model S_i stands for the model constant and N can be equal to 0, 1, 2, and 3, respectively. Depending on choosing the different values of N , four forms of equations can be obtained from Eq. (2). x_B^0 and x_C^0 refer to the initial mole fraction composition of the binary solvent calculated as if solute A was not present. $(x_A)_i$ denotes the saturated mole fraction solubility of the solute in pure solvent i .

When obtaining the model constants with different methods, various variants of the CNIBS/R-K model can be deduced.

Substitution of $(1-x_c^0)$ for x_B^0 in equation with $N=2$ and subse-

quent rearrangements result in Eq. (3).

$$\ln x_A = \ln(x_A)_B + [\ln(x_A)_C - \ln(x_A)_B + S_0 + S_1 + S_2] x_C^0 + [-S_0 + 3S_1 + 5S_2] x_C^{02} + [-2S_1 - 8S_2] x_C^{03} + [-4S_2] x_C^{04} \quad (3)$$

It can also be written as Eq. (4)

$$\ln x_A = B_0 + B_1 x_C^0 + B_2 x_C^{02} + B_3 x_C^{03} + B_4 x_C^{04} \quad (4)$$

In this model, B_0 , B_1 , B_2 , B_3 , and B_4 are parameters, which can be calculated by practical least-squares analysis. Eq. (3) is one form of the variants of CNIBS/R-K model and denotes variant 1 of the CNIBS/R-K model. With Substitution of $(1-x_c^0)$ for x_B^0 in Eq. (2) with $N=2$ and subsequent rearrangement, Eq. (5) can be obtained.

$$\ln x_A - (1-x_c^0) \ln(x_A)_B - x_c^0 \ln(x_A)_C = (1-x_c^0) x_C^0 [S_0 + S_1(1-2x_c^0) + S_2(1-2x_c^0)^2] \quad (5)$$

The parameters S_i could be obtained by regressing.

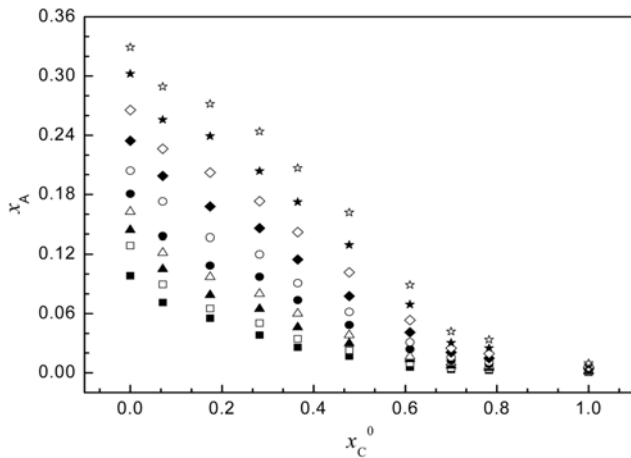


Fig. 2. Experimental solubilities of xylitol in binary ethanol (C)+water (B) solvent mixtures: ■, T=278.00 K; □, T=283.00 K; ▲, T=288.00 K; △, T=293.00 K; ●, T=298.00 K; ○, T=303.00 K; ◆, 308.00 K; ◇, 313.00 K; ★, T=318.00 K; ☆, T=323.00 K. The relative uncertainty for x_A is within 3%.

$$\{\ln x_A - (1-x_C^0)\ln(x_A)_B - x_C^0 \ln(x_A)_C\} \text{ versus } \{(1-x_C^0)x_C^0[S_0+S_1(1-2x_C^0)+S_2(1-2x_C^0)^2]\} \quad (6)$$

This method denotes variant 2 of CNIBS/R-K model, by which the parameters S_0, S_1, S_2 , and calculated solubility can be obtained.

The parameters S_i can also be obtained by regressing

$$\{\ln x_A - (1-x_C^0)\ln(x_A)_B - x_C^0 \ln(x_A)_C / [(1-x_C^0)x_C^0]\} \text{ versus } \{[S_0+S_1(1-2x_C^0)+S_2(1-2x_C^0)^2]\} \quad (7)$$

This method denotes variant 3 of the CNIBS/R-K model.

The experimental solubility data (x_A^{exp}) and back-calculated solubility data ($x_A^{cal.1}, x_A^{cal.2}, x_A^{cal.3}$) are listed in Table 1 by the above three models. The experimental solubility data (x_A^{exp}) also are presented graphically in Fig. 2. The abilities of variant 1, 2, and 3 of CNIBS/R-K model to represent mathematically the experimental solubility of xylitol in binary ethanol+water solvent mixtures at different temperature are summarized in Tables 2-4, respectively, in the form of “curve-fit” parameters and percent deviations in back-calculated

Table 3. Curve-Fitting parameters of xylitol in binary ethanol (C)+water (B) solvent mixtures at the temperature range from 278.00 K to 323.00 K by variant 2

T/K	S_0	S_1	S_2	$\Sigma(\%D)^2$
278.00	2.5460	2.3565	-4.7874	20.620
283.00	2.7660	1.1931	-4.4738	9.6342
288.00	2.5243	1.7451	-5.0630	6.9251
293.00	2.4438	2.4652	-5.5870	10.628
298.00	2.9689	1.6215	-5.1840	5.9222
303.00	3.1402	1.0863	-3.1057	1.9686
308.00	3.2497	1.2541	-3.3095	2.2679
313.00	3.3880	1.1598	-3.4818	4.6696
318.00	3.5553	0.9970	-3.5821	8.5608
323.00	3.6766	0.7538	-3.6446	6.0191
$\Sigma\Sigma(\%D)^2=77.216$				

$\Sigma(\%D)^2$ is the summed squared percentage deviation

solubilities. Summed squared percentage deviation, $\Sigma(\%D)^2$, is calculated by Eq. (8) for assessing the accuracy and predictability of models.

$\Sigma(\%D)^2$ can be defined as:

$$\Sigma(\%D)^2 = \Sigma 100[(x_A^{exp} - x_A^{cal})/x_A^{exp}]^2 \quad (8)$$

Where x_A^{cal} stands for calculated solubility. For overall judgment, sum of $\Sigma(\%D)^2$, i.e. $\Sigma\Sigma(\%D)^2$, is calculated.

Careful examination of Tables 2-4 indicates that three variants provide an accurate mathematical representation for how the solubility of xylitol in binary ethanol+water solvent mixtures at different temperature varies with solvent composition. Comparison of $\Sigma\Sigma(\%D)^2$ for variants 1 and 2, indicated that variant 2 improved the predictability of CNIBS/R-K model about 77%. $\Sigma\Sigma(\%D)^2$ of the variant 1 is far more than variant 2 and variant 3, which means that variant 1 is not adaptable to predict solubility of xylitol in binary ethanol+water system.

3. Thermodynamic Properties for the Solution

According to the previous literature, the thermodynamic properties of the solution process, including the Gibbs energy, enthalpy

Table 2. Curve-Fitting parameters of xylitol in binary ethanol (C)+water (B) solvent mixtures at the temperature range from 278.00 K to 323.00 K by variant 1

T/K	B_0	B_1	B_2	B_3	B_4	$\Sigma(\%D)^2$
278.00	-2.3240	-5.0710	14.561	-35.560	21.571	151.73
283.00	-2.0509	-6.1827	19.264	-40.371	22.771	62.947
288.00	-1.9395	-5.5597	18.593	-39.784	22.538	31.656
293.00	-1.8191	-5.1147	18.924	-42.128	24.371	31.688
298.00	-1.7114	-5.0168	19.143	-40.879	22.825	21.866
303.00	-1.5852	-3.1874	9.6997	-23.500	12.774	2.1061
308.00	-1.4508	-2.9751	10.433	-25.797	14.462	4.5151
313.00	-1.3285	-2.7098	10.211	-24.989	13.634	4.7179
318.00	-1.2013	-2.6811	10.876	-25.507	13.459	10.243
323.00	-1.1137	-2.2438	9.8324	-23.384	12.124	8.2076
$\Sigma\Sigma(\%D)^2=329.68$						

$\Sigma(\%D)^2$ is the summed squared percentage deviation

Table 4. Curve-Fitting parameters of xylitol in binary ethanol (C)+ water (B) solvent mixtures at the temperature range from 278.00 K to 323.00 K by variant 3

T/K	S ₀	S ₁	S ₂	Σ(%D) ²
278.00	2.5460	2.3565	-4.7874	20.620
283.00	2.7660	1.1931	-4.4738	9.6342
288.00	2.5243	1.7452	-5.0631	6.9251
293.00	2.4438	2.4652	-5.587	10.628
298.00	2.9689	1.6215	-5.1839	5.9222
303.00	3.1402	1.0863	-3.1057	1.9686
308.00	3.2497	1.2541	-3.3096	2.2678
313.00	3.3880	1.1598	-3.4818	4.6696
318.00	3.5553	0.9970	-3.5821	8.5608
323.00	3.6766	0.7538	-3.6446	6.0191
ΣΣ(%D) ² =77.215				

Σ(%D)² is the summed squared percentage deviation

and entropy can be calculated by the van't Hoff analysis and defined as [13-15]:

$$\Delta H_{soln}^0 = -R \times \left(\frac{\partial \ln x_i}{\partial (1/T)} \right) \quad (9)$$

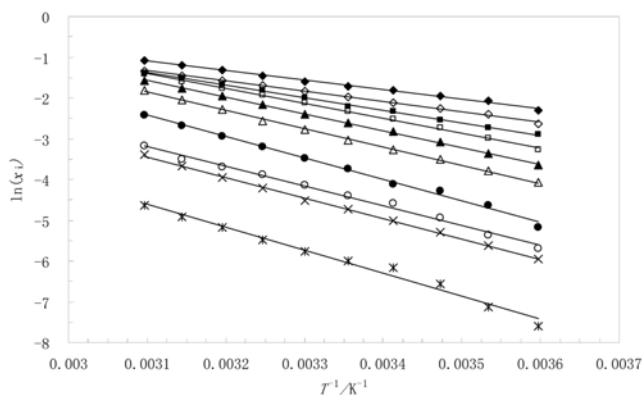
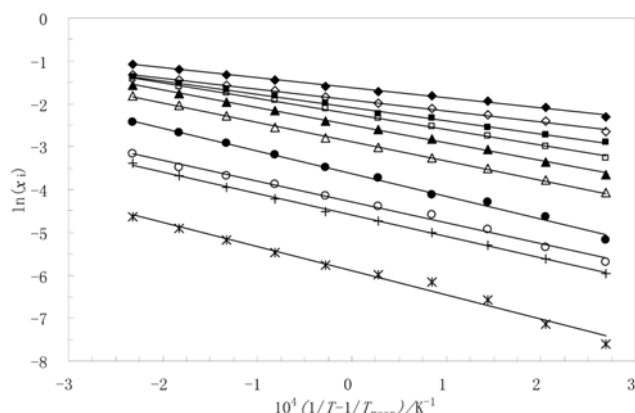
where x is the mole fraction solubility, R represents the universal gas constant (8.314 J·K⁻¹·mol⁻¹) and T is the corresponding absolute temperature. The ΔH_{soln}⁰ can be obtained from the slope of the solubility curve in the so-called van't Hoff plot where ln x_i is plotted versus 1/T.

Over a limited temperature interval, the standard molar enthalpy of solution (ΔH_{soln}⁰) would be valid for the mean temperature, so Eq. (9) can also be written as:

$$\Delta H_{soln}^0 = -R \left(\frac{\partial \ln x_i}{\partial (1/T - 1/T_{mean})} \right) \quad (10)$$

Actually, the derived values of ΔH_{soln}⁰ by Eq. (10) are the same as that by Eq. (9) (Figs. 3 and 4).

The standard molar Gibbs energy of solution (ΔG_{soln}⁰) can be cal-

**Fig. 3.** A van't Hoff plot of the mole fraction solubility (ln(x_i)) of xylitol in solvent mixtures: ◆, x_c⁰=0; ◇, x_c⁰=0.0706; ■, x_c⁰=0.1741; □, x_c⁰=0.2821; ▲, x_c⁰=0.3654; △, x_c⁰=0.4777; ●, x_c⁰=0.6101; ○, x_c⁰=0.7000; ×, x_c⁰=0.7827; ✱, x_c⁰=1.000.**Fig. 4.** Mole fraction solubility (x_i) of xylitol versus temperature (T) in solvent mixtures: ◆, x_c⁰=0; ◇, x_c⁰=0.0706; ■, x_c⁰=0.1741; □, x_c⁰=0.2821; ▲, x_c⁰=0.3654; △, x_c⁰=0.4777; ●, x_c⁰=0.6101; ○, x_c⁰=0.7000; ×, x_c⁰=0.7827; ✱, x_c⁰=1.000.

culated according to literature [16,17]:

$$\Delta G_{soln}^0 = -RT_{mean} \times \text{int except} \quad (11)$$

where the intercept is obtained in plots of ln(x_i) as a function of (1/T - 1/T_{mean}).

Another approach in the literature [18,19] can also be used to estimate ΔS_{soln}⁰ by the equation as follows:

$$\ln x_i = -\frac{\Delta H_{soln}^0}{RT} + \frac{\Delta S_{soln}^0}{R} \quad (12)$$

where ΔS_{soln}⁰ can be calculated from intercept of the solubility curve where ln(x_i) is plotted versus (1/T).

The standard thermodynamic parameters for the solution process in the selected solvent system are listed in Table 5. The standard molar enthalpy of solution for all cases is positive, thereby indicating the solution process of xylitol in each selected solvent is endothermic. For all cases, the standard molar Gibbs energy of solution is positive, which demonstrates that the process is nonspontaneous. The standard molar entropy of solution is positive in all the solvents, which shows that the entropy is the driving force for the

Table 5. Thermodynamic properties of the dissolution of xylitol in different (ethanol+water) mixed solvents: ΔH_{soln}⁰ (kJ·mol⁻¹), ΔG_{soln}⁰ (kJ·mol⁻¹) and ΔS_{soln}⁰ (kJ·mol⁻¹)

x _c ⁰	ΔG _{soln} ⁰	ΔH _{soln} ⁰	ΔS _{soln} ⁰
0.0000	4.0866	19.1279	0.0504
0.0706	4.7646	20.6905	0.0533
0.1741	5.2153	25.0576	0.0664
0.2821	5.5906	29.8339	0.0811
0.3654	6.2624	33.4991	0.0911
0.4777	7.2050	36.3834	0.0976
0.6101	9.0558	42.8841	0.1132
0.7000	10.7372	39.3669	0.0961
0.7827	11.4902	40.7749	0.0983
1.000	14.7441	45.7952	0.1044

x_c⁰ is the mole fraction of ethanol in a mixed solvent

solution process.

cal : calculated
exp : experimental

CONCLUSIONS

From the above analysis, the following accurate conclusions can be drawn: (1) For all selected solvent systems, solubility is a function of temperature and solvent composition. From 278.00 K to 323.00 K, the solubility of xylitol increases with increasing temperature in binary ethanol+water solvent mixtures. (2) At a certain constant temperature, the solubility sharply decreases with increasing ethanol content of the original mixed solvents. (3) The calculated solubility is in good agreement with the experimental values, and the experimental solubility and correlation equation presented in this work can be used as essential data and models in the process of the resolution of xylitol. (4) Variant 2 in the CNIBS/R-K models is more adaptable to predict solubility of xylitol in a binary ethanol+water binary system. (5) The thermodynamic properties for the solution process including Gibbs energy, enthalpy and the entropy were obtained by the van't Hoff analysis and the Gibbs equation.

NOMENCLATURE

A : parameter of the Apelblat equation
B : parameter of the CNIBS model and the Apelblat equation
C : parameter of the Apelblat equation
D : deviation
m : mass
M : molecule weight
N : the number of data points
S : parameter of the CNIBS model
T : temperature
x : molar fraction

Subscripts

A : solute; parameter
B : solvent; parameter
C : anti-solvent

Superscripts

0 : solute not present

REFERENCES

1. B. Rivas, P. Torre, J. M. Dominguez, A. Converti and J. C. Parajo, *J. Agric. Food Chem.*, **54**, 4430 (2006).
2. D. D. Faveri, P. Perego, A. Converti and D. M. Borghi, *J. Chem. Eng.*, **90**, 291 (2002).
3. H. Heikkilae, J. Nygren, M. L. Sarkki, H. Gros, O. P. Eroma, J. Pearson and T. Pepper, *WO Patent*, 9,959,426 (1999).
4. S. M. Payne and F. M. Kerton, *Green Chem.*, **12**, 1648 (2010).
5. G. B. Ren, J. K. Wang, Q. X. Yin and M. J. Zhang, *J. Chem. Eng. Data*, **49**, 1671 (2004).
6. S. Wang, J. K. Wang, Q. X. Yin and Y. L. Wang, *Chin. Opt. Lett.*, **3**, 149 (2005).
7. S. Wang, J. K. Wang and Q. X. Yin, *Ind. Eng. Chem. Res.*, **44**, 3783 (2005).
8. H. X. Hao, J. K. Wang and Y. L. Wang, *J. Chem. Eng. Data*, **49**, 697 (2004).
9. D. Q. Li, D. Z. Liu and F. A. Wang, *J. Chem. Eng. Data*, **46**, 234 (2001).
10. W. E. Acree, *J. Thermochim. Acta*, **198**, 71 (1992).
11. W. E. Acree, J. McCargar, J. W. Zvaigzne and A. L. Teng, *Phys. Chem. Liq.*, **23**, 27 (1991).
12. W. E. Acree and J. W. Zvaigzne, *J. Thermochim. Acta*, **178**, 151 (1991).
13. A. Maher, D. Croker, A. C. Rasmuson and B. K. Hodnett, *J. Chem. Eng. Data*, **55**, 5314 (2010).
14. D. W. Wei, H. Li, Y. N. Li and J. Zhu, *Fluid Phase Equilib.*, **316**, 132 (2012).
15. B. Schroder, L. M. N. B. F. Santos, I. M. Marrucho and J. A. P. Coutinho, *Fluid Phase Equilib.*, **289**, 140 (2010).
16. M. A. Ruidiaz, D. R. Delgado, F. Martinez and Y. Marcus, *Fluid Phase Equilib.*, **299**, 259 (2010).
17. X. Q. Zhou, J. S. Fan, N. Li, Z. X. Du, H. J. Ying, J. L. Wu, J. Xiong and J. X. Bai, *Fluid Phase Equilib.*, **316**, 26 (2012).
18. W. S. Choi and K. J. Kim, *J. Chem. Eng. Data*, **56**, 43 (2010).
19. P. Wang, J. K. Wang, J. B. Gong and M. J. Zhang, *Fluid Phase Equilib.*, **306**, 171 (2011).