

Thermodynamic Models for Determination of the Solubility of N-Acetylglycine in (Methanol+Acetonitrile) Binary Solvent Mixtures

Wangdan Zhao¹, Wenge Yang^{1*}, Qirun Guo¹, Shimin Fan¹, Jianfeng Hao¹ and Yonghong Hu²

¹School of Pharmaceutical Sciences, Nanjing Tech University, No. 30, South Puzhu Road, Nanjing 211816, PR China

²State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing Tech University, No.200, North Zhongshan Road, Nanjing 210009, PR China

Abstract

N-Acetylglycine is an important organic chemical and pharmaceutical intermediate. The solubility of N-Acetylglycine in methanol+Acetonitrile was measured in the temperature ranging from 278.15 K to 333.15 K. In the processing of the experimental data, we use three kinds of equations. There are the Combined Nearly Ideal Binary Solvent/Redlich–Kister (CNIBS/R–K) equations and the simplified Jouyban–Acree equation. All equations can be well applied. The CNIBS/R–K equations are relatively better. We used the van't Hoff equation to determine the thermodynamic properties of N-Acetylglycine further more, including the entropy, enthalpy, and Gibbs energy.

Keywords: N-Acetylglycine; Solubility-temperature dependence; Pharmaceutical intermediate; Correlation; Enthalpy; Jouyban–Acree equation; CNIBS/R–K equation

Introduction

N-Acetylglycine (Figure 1, CAS: 543-24-8, MW=117.10) is a long needle crystal and its crystal structure has been reported in the literature [1,2]. N-Acetylglycine is important organic chemical intermediate for many chemical products, such as glycine, aspartame and other amino acids. It is also important pharmaceutical intermediate for Acetyl glutamine that can be used for the patient to promote department of neurosurgery coma after surgery. N-Acetylglycine was widely used in pharmaceutical [3], pesticide [4], chemical industry [5] and other fields. N-Acetylglycine is prepared from paraformaldehyde; acetamide, carbon monoxide with a catalyst system, then gained with concentrating and filtrating, and can be purified by crystallization (Figure 2). Therefore, to know the relationship between N-Acetylglycine solubility with temperature and solvent composition is very important for the preparation and purification of products. As far as we know, it has not been reported about the solubility data of N-Acetylglycine in (methanol+Acetonitrile) mixtures. So we provided the helpful and valuable information on the crystallization of N-Acetylglycine. We chose methanol and acetonitrile as the binary solvent mixtures system in this paper. The reason to make such a choice is that the solubility of N-Acetylglycine in methanol is better than acetonitrile in previous study. In this paper, the solubility of N-Acetylglycine in methanol+Acetonitrile mixtures was determined between 278.15 K and 333.15 K at standard atmospheric pressure (101.325 kPa) by the dynamic method. The experimental data measured was correlated with two forms of Redlich–Kister (CNIBS/R–K) equation and the simplified Jouyban–Acree equation. The thermodynamic properties of the solution process, including the Gibbs energy, enthalpy, and entropy, were calculated by the van't Hoff analysis.

Experimental

Materials and apparatus

All solvents and N-Acetylglycine (Aladdin Chemistry Co., Ltd) used for experiments were of analytical reagent grade and their mass fraction purities were higher than 99%. More details about the purity of reagents are listed in Table 1. Analytical balance (model: BSA224S) was provided from Sartorius Scientific Instruments (Beijing) CO., Ltd.

with an uncertainty of ± 0.0002 g. The smart Acetonitrile-circulator thermostatic bath (model: DC-2006) was provided by Ningbo Scientz Biotechnology Co. Ltd. with an uncertainty of ± 0.1 K.

Methods

The solubility of N-Acetylglycine in methanol+Acetonitrile mixtures was determined from 278.15 K to 333.15 K at atmospheric pressure by the dynamic method [6-8]. Solvents and excess N-Acetylglycine were added into glass test tubes with stoppers. The glass test tubes were maintained at a double layer jacket glass equilibrium cell which was full of solution. The temperature of the inner was controlled by circulating which was from a smart Acetonitrile-circulator thermostatic bath. Stirring the mixture continuously used a magnetic stirrer for twentyfour hours until it reaching saturation and equilibrium. Then stop stirring to let the solution settle over nights to make sure the suspended solid precipitated. Next, took 1 mL the clear upper saturated solution by a pipette gun and transferred it into a 10 mL beaker with a cover that had been weighed up beforehand

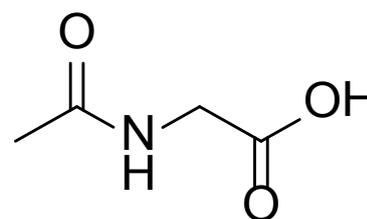


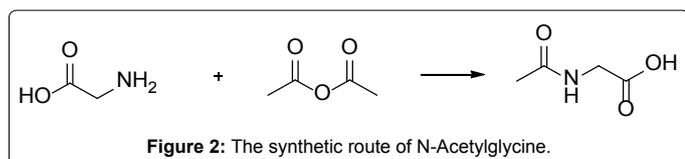
Figure 1: Chemical structure of N-Acetylglycine.

*Corresponding author: Wenge Yang, School of Pharmaceutical Sciences, Nanjing Tech University, No. 30, South Puzhu Road, Nanjing 211816, PR China, E-mail: wengeyang11@163.com

Received April 23, 2016; Accepted May 10, 2016; Published May 25, 2016

Citation: Zhao W, Yang W, Guo Q, Fan S, Hao J, et al. (2016) Thermodynamic Models for Determination of the Solubility of N-Acetylglycine in (Methanol+Acetonitrile) Binary Solvent Mixtures. J Thermodyn Catal 7: 166. doi:10.4172/2160-7544.1000166

Copyright: © 2016 Zhao W, et al. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.



Compound	Provenance	Mass fraction purity
N-Acetylglycine	Aladdin Chemistry	0.990
Methanol	Aladdin Chemistry	0.996
Acetonitrile	Aladdin Chemistry	0.991

Table 1: Provenance and purity of the materials used.

and then measured the total weight rapidly. Then the beaker was put into a dryer and the mass was recorded repeatedly until keeping the constant weight. Each experiment was repeated at least three times and we used the average value to calculate the mole fraction solubility at last. The mole fraction solubility of N-Acetylglycine (x_i) in methanol+Acetonitrile is calculated by equation (1). The composition of solvent mixtures (x_{II}) is defined using equation (2).

$$x_i = \frac{m_i/M_i}{m_i/M_i + m_{II}/M_{II} + m_{III}/M_{III}} \quad (1)$$

$$x_{II} = \frac{m_{II}/M_{II}}{m_{II}/M_{II} + m_{III}/M_{III}}, x_{III} = \frac{m_{III}/M_{III}}{m_{II}/M_{II} + m_{III}/M_{III}} \quad (2)$$

where m_i , m_{II} , m_{III} represent the mass of the solute, methanol, Acetonitrile, and M_i , M_{II} , M_{III} represent the molecular weight of the solute, methanol, Acetonitrile, respectively.

Results and Discussion

Solubility data

The solubility data (x_i) of N-Acetylglycine in methanol+Acetonitrile mixtures with the temperature ranging from 278.15 to 333.15 K are presented in Table 2. For comparison with each of the experimental points, experimental solubility data of N-Acetylglycine in methanol+Acetonitrile mixtures in the temperature range from 278.15 to 333.15 K are presented in Figures 3 and 4. From Table 2 and Figure 3, it can be found that the solubility of N-Acetylglycine in methanol+Acetonitrile mixtures is a function of temperature and solvent composition. More specifically, the solubility of N-Acetylglycine in Methanol+Acetonitrile mixtures increases with the rise of temperature, while at a constant temperature increases with increasing methanol content of the mixed solvent. By these properties, methanol could be used as effective benign solvent in the crystallization process.

Data correction

The relationship of the experimental isothermal mole fraction solubility and binary solvent compositions is described by the Combined Nearly Ideal Binary Solvent /Redlich-Kister (CNIBS/R-K) model [9-11]. The model is presented in equation (3).

$$\ln x_i = x_{II} \ln(x_i)_{II} + x_{III} \ln(x_i)_{III} + x_{II}x_{III} \sum_{i=0}^N S_i(x_{II} - x_{III})^i \quad (3)$$

Where x_{II} and x_{III} represent the initial mole fraction composition of the binary solvent when the solute was not added. S_i is the model constant and the value of N can be 0, 1, 2 and 3. $(x_i)_i$ represents the saturated mole fraction solubility of the solute(N-Acetylglycine) in pure solvent i . When $N=2$ and substitution of $(1-x_{II})$ for x_{III} , then equation (3) can be converted into equation (4).

$$\ln x_i = \ln(x_i)_{III} + (\ln(x_i)_{II} - \ln(x_i)_{III}) + (S_0 - S_1 + S_2)x_{II} + (-S_0 + 3S_1 - 5S_2)x_{II}^2 + (-2S_1 + 8S_2)x_{II}^3 + (-4S_2)x_{II}^4 \quad (4)$$

Which can be further simplified as the following equation:

$$\ln x_i = C_0 + C_1x_{II} + C_2x_{II}^2 + C_3x_{II}^3 + C_4x_{II}^4 \quad (5)$$

where C_0 , C_1 , C_2 , C_3 , C_4 are model constants and we can get these constants by least-squares analysis [12].

Equation (5) is just variant one of CNIBS/R-K model. When $N=2$ and x_{III} is relaced by $(1-x_{II})$, equation (3) can rearrangements result in equation (6).

This is variant two of CNIBS/R-K model [10]. The parameters S_i would be obtained by regressing

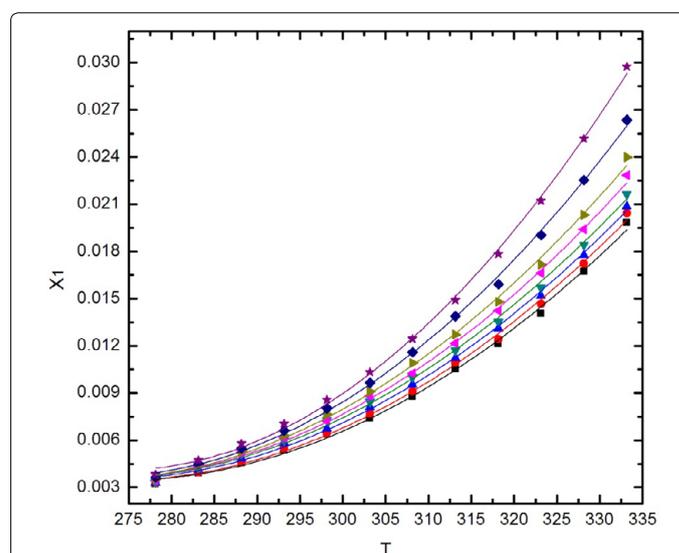


Figure 3: Solubility of N-Acetylglycine in Methanol+Acetonitrile binary solvent mixtures: \blacksquare , $x_{II}=0$; \bullet , $x_{II}=9.027\%$; \blacktriangle , $x_{II}=19.419\%$; \blacktriangledown , $x_{II}=31.510\%$; \blacktriangleleft , $x_{II}=45.754\%$; \blacktriangleright , $x_{II}=62.782\%$; \blacklozenge , $x_{II}=83.500\%$; \star , $x_{II}=1$.

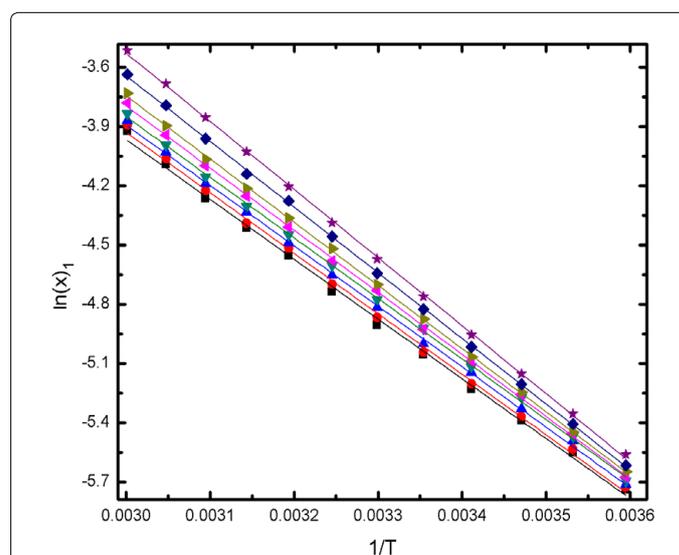


Figure 4: Mole fraction solubility ($\ln(x_i)$) of N-Acetylglycine in the binary solvent against $1/T$ with a straight line to correlate the data: \blacksquare , $x_{II}=0$; \bullet , $x_{II}=9.027\%$; \blacktriangle , $x_{II}=19.419\%$; \blacktriangledown , $x_{II}=31.510\%$; \blacktriangleleft , $x_{II}=45.754\%$; \blacktriangleright , $x_{II}=62.782\%$; \blacklozenge , $x_{II}=83.500\%$; \star , $x_{II}=1$.

x_i	$100x_i$	$100(x_i - x_i^{cal})/x_i$ (Eq. 5)	$100(x_i - x_i^{cal})/x_i$ (Eq. 6)	$100(x_i - x_i^{cal})/x_i$ (Eq. 9)
T=278.15 K				
0.000	0.322	-0.086	0.000	-1.266
0.090	0.326	0.168	0.221	-0.042
0.194	0.330	-0.013	-0.057	1.249
0.315	0.336	-0.088	-0.091	0.098
0.458	0.343	-0.091	-0.074	-0.140
0.628	0.352	0.197	0.194	0.097
0.835	0.364	-0.116	-0.119	-0.032
1.000	0.384	0.029	0.000	0.004
T=283.15 K				
0.000	0.389	0.474	0.000	-2.558
0.090	0.395	-1.098	-1.172	-0.974
0.194	0.412	0.531	0.468	3.340
0.315	0.421	0.264	0.402	0.003
0.458	0.427	0.049	0.051	-0.005
0.628	0.431	-0.498	-0.604	0.003
0.835	0.449	0.346	0.417	-0.002
1.000	0.473	-0.091	0.000	0.000
T=288.15 K				
0.000	0.457	0.472	0.000	-2.649
0.090	0.465	-1.093	-1.023	-0.975
0.194	0.484	0.530	-0.569	3.421
0.315	0.513	0.265	1.501	0.015
0.458	0.521	0.039	-0.110	-0.021
0.628	0.527	-0.483	-1.012	0.016
0.835	0.549	0.338	0.707	-0.005
1.000	0.579	-0.089	0.000	0.001
T=293.15 K				
0.000	0.536	0.487	0.000	-3.817
0.090	0.550	-1.097	-1.309	-1.004
0.194	0.582	0.495	0.577	4.428
0.315	0.601	0.309	0.394	0.122
0.458	0.616	-0.015	-0.039	-0.173
0.628	0.630	-0.418	-0.490	0.121
0.835	0.663	0.298	0.353	-0.039
1.000	0.705	-0.077	0.000	0.005
T=298.15 K				
0.000	0.638	0.438	0.000	-3.746
0.090	0.646	-0.952	-1.406	-0.875
0.194	0.673	0.342	-0.872	4.238
0.315	0.728	0.399	2.863	0.172
0.458	0.724	-0.072	-1.743	-0.244
0.628	0.764	-0.373	-0.069	0.171
0.835	0.803	0.275	0.375	-0.055
1.000	0.856	-0.072	0.000	0.007
T=203.15 K				
0.000	0.741	0.481	0.000	-4.786
0.090	0.769	-1.075	-0.440	-1.026
0.194	0.809	0.515	0.206	5.251
0.315	0.843	0.218	-0.099	0.131
0.458	0.883	0.048	0.420	-0.182
0.628	0.909	-0.410	-0.503	0.126
0.835	0.964	0.274	0.251	-0.040
1.000	1.034	-0.069	0.000	0.005
T=308.15 K				
0.000	0.876	0.501	0.000	-4.998
0.090	0.910	-1.100	-0.543	-1.082
0.194	0.954	0.511	0.023	5.489
0.315	1.002	0.182	0.876	0.071

0.458	1.025	0.155	-0.982	-0.098
0.628	1.090	-0.506	0.443	0.068
0.835	1.159	0.314	-0.098	-0.021
1.000	1.245	-0.078	0.000	0.004
T=313.15 K				
0.000	1.052	0.490	0.000	-5.047
0.090	1.094	-1.117	0.208	-1.040
0.194	1.122	0.533	-0.621	5.473
0.315	1.172	0.231	0.416	0.141
0.458	1.216	0.056	0.260	-0.195
0.628	1.273	-0.416	-0.456	0.134
0.835	1.389	0.275	0.220	-0.042
1.000	1.492	-0.069	0.000	0.005
T=318.15 K				
0.000	1.212	0.024	0.000	-2.710
0.090	1.241	-0.053	-0.757	-0.281
0.194	1.311	0.186	0.790	2.975
0.315	1.353	-0.553	-0.433	-0.500
0.458	1.423	0.760	0.249	0.678
0.628	1.480	-0.531	-0.197	-0.453
0.835	1.592	0.190	0.097	0.134
1.000	1.782	-0.036	0.000	-0.015
T=323.15 K				
0.000	1.384	-0.335	0.000	-3.300
0.090	1.406	0.716	0.192	0.505
0.194	1.465	-0.127	-0.128	2.700
0.315	1.517	-0.707	-0.592	-0.297
0.458	1.568	0.517	1.164	0.403
0.628	1.662	-0.013	-0.895	-0.266
0.835	1.717	-0.089	0.326	0.079
1.000	1.904	0.026	0.000	-0.008
T=328.15 K				
0.000	1.673	0.033	0.000	-3.006
0.090	1.723	0.052	0.043	-0.024
0.194	1.776	-0.181	-0.178	2.962
0.315	1.843	-0.164	-0.156	-0.365
0.458	1.941	0.660	0.652	0.495
0.628	2.032	-0.601	-0.599	-0.327
0.835	2.254	0.240	0.240	0.095
1.000	2.516	-0.048	0.000	-0.010
T=333.15 K				
0.000	1.982	-0.042	0.000	-2.843
0.090	2.043	0.108	0.693	-0.110
0.194	2.085	0.063	-0.345	2.782
0.315	2.163	-0.501	-0.434	0.044
0.458	2.283	0.677	0.514	-0.060
0.628	2.399	-0.432	-0.164	0.040
0.835	2.636	0.142	-0.001	-0.011
1.000	2.975	-0.026	0.000	0.001

*Standard uncertainties u are $u(T)=0.1\text{K}$, $u(x_I)=0.0002$, $u(p)=0.02$

Table 2: Mole fraction solubility (x_I) of N-Acetylglucine in Methanol+Acetonitrile binary solvent mixtures at the temperature range from (278.15 to 333.15) K under atmospheric pressure^a.

$$\{\ln x_I - (1 - x_{II}) \ln(x_I)_{III} - x_{II} \ln(x_I)_{II}\} \text{ Versus } \{(1 - x_{II})x_{II}[S_0 + S_1(2x_{II} - 1) + S_2(2x_{II} - 1)^2]\} \quad (6)$$

The CNIBS/R-K model only can be used to describe the solubility data and to predict solubility data for different concentrations of a mixed

solvent at a fixed temperature. To describe the effect of both solvent compositions and temperature on the solubility of N-Acetylglucine, another model called Jouyban-Acree model was adopted [12,13]

$$\ln x_I = x_{II} \ln(x_I)_{II} + x_{III} \ln(x_I)_{III} + x_{II}x_{III} \sum_{i=0}^N \frac{J_i(x_{II} - x_{III})^i}{T} \quad (7)$$

where J_1 is the model constant, T is the absolute temperature, and other symbols denote the same meaning as equation (3). When $N=2$ and x_{III} is replaced by $(1-x_{II})$ in equation (7), we can obtain equation (8) after rearrangement.

$$\ln x_I = \ln(x_I)_{III} + (\ln(x_I)_{II} - \ln(x_I)_{III})x_{II} + \frac{(J_0 - J_1 + J_2)x_{II}}{T} + \frac{(-J_0 + 3J_1 - 5J_2)x_{II}^2}{T} + \frac{(-2J_1 + 8J_2)x_{II}^3}{T} + \frac{(-4J_2)x_{II}^4}{T} \quad (8)$$

Equation (8) can also be further simplified as another form:

$$\ln x_I = D_0 + D_1/T + D_2 \ln T + D_3 x_{III} + [D_4 x_{III} + D_5 x_{III}^2 + D_6 x_{III}^3 + D_7 x_{III}^4]/T + D_8 x_{III} \ln T \quad (9)$$

where $D_0, D_1, D_2, D_3, D_4, D_5, D_6, D_7, D_8$ are parameters of this model.

Experimental solubility data of N-Acetylglycine were correlated with equation (5), equation (6) and equation (9). Calculated solubility data (x_I^{cal}) from these models are listed in Table 2.

The mean deviation (MD) [14,15] used as the validity of the models is introduced and calculated by equation (10):

$$MD = 100 \frac{\sum |x_I - x_I^{cal}|}{N} \quad (10)$$

where N is the number of experimental points, x_I is the experimental solubility and x_I^{cal} is the calculated solubility. The parameter values of equation (5), equation (6) and equation (9) are listed in Tables 3-5 together with the values of MD.

As we can see from Tables 3-5, obtained overall MD value for the variant 1 of CNIBS/R-K equation is 0.384, for the variant 2 of CNIBS/R-K equation is 0.377, and for the Jouyban-Acree equation is 1.042. This result indicated that the experimental data agreed well with the calculated results from the three equations, and the the variant 2 of CNIBS/R-K equation provided the more accurate prediction according to its lower value of the overall MD. The CNIBS/R-K equation can only be used for the prediction of solubility for different concentrations of a mixed solvent at constant temperature, while the Jouyban-Acree equation can be used for predicting solubility at different temperatures and different concentrations.

Thermodynamic analysis of dissolution

We can calculate the standard molar enthalpy of dissolution (ΔH_{soln}^0) from the slope of the $\ln x_I$ versus $1/T$ plot by equation (11). This is the van't Hoff analysis and it is defined as [16-18]:

$$\Delta H_{soln}^0 = -R \times \left(\frac{\partial \ln x_I}{\partial (1/T)} \right) \quad (11)$$

The standard molar enthalpy of dissolution (ΔH_{soln}^0) would be valid for the mean temperature ($T_{mean} = 305.65$ K, in the present work) in a certain temperature range. Equation (11) can also be represented as:

$$\Delta H_{soln}^0 = -R \times \left(\frac{\partial \ln x_I}{\partial (1/T - 1/T_{mean})} \right) \quad (12)$$

In addition, we can also calculate the standard molar Gibbs energy

of dissolution (ΔG_{soln}^0) according to [19]:

$$\Delta G_{soln}^0 = -RT_{mean} \times intercept \quad (13)$$

where the intercept is obtained in plots of $\ln x_I$ versus $(1/T - 1/T_{mean})$.

Then the standard molar entropy of dissolution (ΔS_{soln}^0) is calculated by [20]:

$$\Delta S_{soln}^0 = \frac{\Delta H_{soln}^0 - \Delta G_{soln}^0}{T_{mean}} \quad (14)$$

The calculation results of the standard Gibbs energy, enthalpy, and entropy are shown in Tables 6 together with ξ_{TS} and ξ_H . The ξ_{TS} and ξ_H is the comparison of the relative contribution to the standard Gibbs energy by enthalpy and entropy in the dissolution process, respectively.

$$\% \xi_H = \frac{|\Delta H_{soln}^0|}{|\Delta H_{soln}^0| + |T \Delta S_{soln}^0|} \times 100 \quad (15)$$

$$\% \xi_{TS} = \frac{|T \Delta S_{soln}^0|}{|\Delta H_{soln}^0| + |T \Delta S_{soln}^0|} \times 100 \quad (16)$$

We can conclude from Table 6 that the standard Gibbs energy and the enthalpy of N-Acetylglycine are positive in the selected binary solvent mixtures, so it means the dissolution process of N-Acetylglycine in Methanol+Acetonitrile is endothermic. Furthermore, the main contributor to the standard molar Gibbs energy of solution is the enthalpy during the dissolution in virtue of values of $\% \xi_H$ are ≥ 64.038 for Methanol+Acetonitrile.

Conclusions

In this work new data were provided for the solubility of

T/K	C ₀	C ₁	C ₂	C ₃	C ₄	MD
278.15	-5.738	0.080	0.349	-0.665	0.412	0.099
283.15	-5.555	0.387	-0.469	0.129	0.154	0.419
288.15	-5.358	0.396	-0.466	0.107	0.170	0.514
293.15	-5.235	0.529	-0.566	0.138	0.180	0.399
298.15	-5.042	0.507	-0.469	0.001	0.243	0.665
303.15	-4.910	0.632	-0.627	0.128	0.205	0.486
308.15	-4.742	0.648	-0.562	0.004	0.267	0.419
313.15	-4.559	0.663	-0.662	0.158	0.195	0.399
318.15	-4.413	0.256	0.251	-0.612	0.492	0.391
323.15	-4.261	0.296	0.062	-0.362	0.412	0.316
328.15	-4.091	0.327	-0.030	-0.106	0.219	0.248
333.15	-3.896	0.321	-0.239	0.261	0.039	0.249
					Overall	MD=0.384

Table 3: Parameters the variant 1 of CNIBS/R-K equation for N-Acetylglycine in Methanol+Acetonitrile binary solvent mixtures at the temperature range from (278.15 to 333.15) K.

T/K	S ₀	S ₁	S ₂	MD
278.15	-0.073	-0.083	-0.091	0.095
283.15	-0.001	-0.204	-0.067	0.389
288.15	0.085	-0.191	-0.234	0.615
293.15	0.039	-0.228	-0.068	0.395
298.15	0.030	-0.123	-0.187	0.916
303.15	0.059	-0.198	-0.122	0.240
308.15	0.011	-0.152	0.003	0.371
313.15	-0.082	-0.109	0.082	0.273
318.15	-0.094	-0.250	-0.231	0.315
323.15	-0.151	-0.233	-0.020	0.412
328.15	-0.194	-0.164	-0.054	0.234
333.15	-0.214	-0.174	-0.137	0.269
			Overall	MD= 0.377

Table 4: Parameters the variant 2 of CNIBS/R-K equation for N-Acetylglycine in Methanol+Acetonitrile binary solvent mixtures at the temperature range from (278.15 to 333.15) K.

T/K	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	MD
278.15										0.366
283.15										0.861
288.15										0.888
293.15										1.214
298.15										1.188
303.15										1.443
308.15										1.479
313.15										1.510
318.15										0.968
323.15										0.945
328.15										0.911
333.15										0.736
	-1.281	-61.475	-6.620	-0.070	6.742	11.842	15.437	9.908	1.191	
									Overall	MD=1.042

Table 5: Parameters of the Jouyban-Acree equation for N-Acetylglycine in Methanol+Acetonitrile binary solvent mixtures at the temperature range from (278.15 to 333.15) K.

x_{II}	$\Delta H_{so}^0 / \text{KJ}\cdot\text{mol}^{-1}$	$\Delta G_{so}^0 / \text{KJ}\cdot\text{mol}^{-1}$	$\Delta S_{so}^0 / \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$\% \xi_H$	$\% \xi_{TS}$
0.000	22.869	12.381	34.944	68.558	31.442
0.090	23.270	12.314	36.503	67.989	32.011
0.194	23.494	12.212	37.587	67.559	32.441
0.315	23.671	12.110	38.516	67.187	32.813
0.458	24.266	12.038	40.739	66.493	33.507
0.628	24.713	11.954	42.509	65.951	34.049
0.835	25.648	11.802	46.128	64.942	35.058
1.000	26.508	11.621	49.596	64.038	35.962

Table 6: Thermodynamic functions relative to solution process of N-Acetylglycine in Methanol+Acetonitrile binary solvent mixtures at mean temperature.

N-Acetylglycine in Methanol+Acetonitrile mixtures at temperature range from 278.15 K to 333.15 K. We can draw the following conclusions: The solubility of N-Acetylglycine in Methanol+Acetonitrile mixtures increases with the rise of temperature, while at a constant temperature increased with increasing methanol content of the mixed solvent. The solubility data could be successfully correlated using the two variants of the combined nearly ideal binary solvent/Redlich-Kister (CNIBS/R-K) equation and the Jouyban-Acree equation, but the variant 2 of CNIBS/R-K equation was more accurate than the other two equations. The thermodynamic properties for the dissolution process including Gibbs energy, enthalpy, and entropy were obtained by the van't Hoff analysis. The enthalpy change and the standard Gibbs energy change are positive proved that the dissolution process of N-Acetylglycine in Methanol+Acetonitrile mixtures was endothermic and contributor to the standard molar Gibbs energy of solution was the enthalpy during the dissolution due to values of $\% \xi_H$ are ≥ 64.038 . The experimental solubility data and the parameters could be used for optimizing the purification process of N-Acetylglycine in industry.

Acknowledgements

This research work was financially supported by the Science and Technology support program of Jiangsu Province (Agriculture) (Grant No. BE2012373, BE2012374), the College Industrialization Project of Jiangsu Province (Grant No. JHB2011-16).

References

- Karpenter GB, Donohue J (1950) The Crystal Structure of N-Acetylglycine. J Am Chem Soc 72: 2315-2328.
- Donohue J, Marsh RE (1962) A refinement of the structure of N-acetylglycine. Acta Cryst 15: 941.
- Asiago VM, Alvarado LZ, Shanaiah N, Gowda GA, Owusu-Sarfo K, et al. (2010) Early detection of recurrent breast cancer using metabolite profiling. Cancer Res 70: 8309-8318.
- Kim SK, Ubukata M, Isono K (2003) N-Acetylglycine side chain is critical for the antimicrobial activity of xanthostatin. Journal of Microbiology and Biotechnology 13: 998-1000.
- Harburn JJ, Rath NP, Spilling CD (2005) Efficient synthesis of tyrosine-derived marine sponge metabolites via acylation of amines with a coumarin. J Org Chem 70: 6398-6403.
- Hu YH, Chen X, Yang WG, Guan J (2009) Measurement and correlation of the solubility of urea l-tartaric acid in aqueous ethanol solution. Thermochim Acta 484: 38-40.
- Chen ZG, Yang WG, Hu YH, Lei ZY (2011) J Chem Eng Data 56: 2676-2679.
- Lei ZY, Hu YH, Yang WG, Li L (2011) Solubility of 2-(2, 4, 6-trichlorophenoxy) ethyl bromide in methanol, ethanol, propanol, isopropanol, acetonitrile, n-heptane, and acetone. J Chem Eng Data 56: 2714-2719.
- Wang JY, Lee LN, Lai HC, Wang SK, Jan IS, et al. (2007) Fluoroquinolone resistance in Mycobacterium tuberculosis isolates: associated genetic mutations and relationship to antimicrobial exposure. J Antimicrob Chemother 59: 860-865.
- Wang P, Jiang JX, He LT, Li HQ, Li J, et al. (2013) Solubility of isomalt in the water+ethanol solvent system at (288.15, 298.15, 308.15, and 318.15) K. J Chem Eng Data 58: 364-369.
- Noubigh A, jeribi C, Mgaidi A, Abderrabba M (2012) Solubility of gallic acid in liquid mixtures of (ethanol+ water) from (293.15 to 318.15) K. J Chem Thermodynamics 55: 75-78.
- Sun H, Li M, Jia JT, Tang FK, Duan EH (2012) Measurement and correlation of the solubility of 2, 6-diaminohexanoic acid hydrochloride in aqueous methanol and aqueous ethanol mixtures. J Chem Eng Data 57: 1463-1467.
- Hasana M, Sawanta AB, Sawanta RB, Loke PG (2011) Densities, viscosities, speed of sound, and IR spectroscopic studies of binary mixtures of tert-butyl acetate with benzene, methylbenzene, and ethylbenzene at T=(298.15 and 308.15) K. J Chem Thermodynamics 43: 1389-1394.
- Zhao Y, Wang YI (2013) J Chem Thermodynamics 57: 9-13.
- Lim J, Jang S, Cho HK, Shin MS, Kim H (2013) Solubility of salicylic acid in pure alcohols at different temperatures. J Chem Thermodynamics 57: 295-300.
- Wang S, Qin LY, Zhou ZM, Wang JD (2012) Solubility and solution thermodynamics of betaine in different pure solvents and binary mixtures. J Chem Eng Data 57: 2128-2135.
- Wei DW, Li H, Li YN, Zhu J (2012) Effect of temperature on the solubility of 3-aminopyridine in binary ethanol+ toluene solvent mixtures. J Fluid Phase Equilibria 316: 132-134.
- Maher A, Croker D, Rasmuson AC, Hodnett BK (2010) Solubility of Form III Piracetam in a Range of Solvents. J Chem Eng Data 55: 5314-5318.
- Zhou XQ, Fan JS, Li N, Du ZX, Ying HJ, et al. (2012) Solubility of l-phenylalanine in water and different binary mixtures from 288.15 to 318.15 K. Fluid Phase Equilibria. 316: 26-33.
- Azara VP, Ahmadian S, Martínez F, Acree Jr WE, Jouyban A (2012) Thermodynamic studies of fluphenazine decanoate solubility in PEG 200+ water mixtures. Fluid Phase Equilibria 330: 36-43.