Determination and Correlation of the Solubility for Taurine in Water and Organic Solvent Systems

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Using a laser monitoring technique, the solubility data of taurine in water and aqueous solutions of methanol, ethanol, and 2-propanol were measured over the temperature range from (274.05 to 353.05) K. From the experimental data, the solubility data of taurine in the mixtures of water + methanol, water + ethanol, and water + 2-propanol were found to increase with increasing temperature and decrease with increasing concentration of methanol, ethanol, and 2-propanol in aqueous solution. Also, the water + ethanol solution was a better solvent for the purification of taurine. The Apelblat equation, the simplified model of ideal solution, and the λh equation were used to correlate the solubility data; the results showed that the three models mentioned above agreed well with the experimental data, and the Apelblat equation was the most accurate of all of these for these systems.

Introduction

Taurine (2-aminothanesulfonic acid, CAS Registry No. 107-35-7) is an essential sulfur-containing nonprotein amino acid, which is one of the most abundant among low molecular weight organic constituents in the brain and heart of many animals, including mammals, and an essential nutrient in the growth of newborns and infants. A variety of physiological functions, pharmacological actions, and pathological conditions seem to be regulated by taurine.[1]

The techniques of preparing taurine have been largely developed in industry. The preparation of taurine with ethanolamine, H_2SO_4, and sodium sulfite as raw materials[2] is one of the interesting techniques. However, we face difficulties by using an effective method of isolating taurine from the mixture of impurities. The crystallization of taurine in water is the most frequently used method, but it has yet to be heightened in the yield and purification. Now, it has been reported that the crystallization technology of using an aqueous solution of ethanol for the crystallization of taurine is an interesting method.[3,4] To gain high-yield purification of taurine and be available to explore new synthesis methods, engineering design, and industry productions of taurine, the solubility data of taurine in water + methanol, water + ethanol, and water + 2-propanol systems at different temperatures were investigated by using laser monitoring technology in this paper, and the experimental data were correlated with Apelblat equation, the simplified model of ideal solution, and the λh equation.

Experimental Section

Materials. Taurine (mass fraction purity of 0.994) was purchased from Zhengzhou Friend Living Creature Engineering Co. Ltd., China. Absolute ethyl alcohol, methanol, 2-propanol, benzoic acid, and sodium sulfate used in the experiment were of AR grade with a mass fraction purity of over 0.995 and were purchased from Laiyang Shuangshuang Co. Ltd., China. Distilled−deionized water was used.

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Procedure. The solubility data of a solid in solvent were determined by a synthetic method.[5−7] The solubility apparatus and method were the same as in our former work.[8] To check the reliability of the measurement, a comparison of solubility data for both sodium sulfate and benzoic acid in water between experimental values and literature values[9,10] was made in Figure SI 1 (Supporting Information, SI). The average relative deviation in the mole fraction solubility of above two systems was 0.02, and the standard uncertainty of determination for the mole fraction solubility was 0.0001. So it had been proven that this experimental technique was reliable.

Results and Discussion

The solubility data of taurine in water and the mixture of water and methanol, ethanol, or 2-propanol were determined by laser monitoring technology[11] in the temperature range of (274.05 to 353.05) K. The solubility data from the experiment were correlated with Apelblat equation, the simplified model of ideal solution, and the λh equation,[8,11] which are shown as follows, respectively:

$$\ln x = A + \frac{B}{T} + C \ln T \tag{1}$$

$$\ln x = \frac{A'}{T} + B' \tag{2}$$

Table 1. Mole Fraction Solubility x of Taurine Obtained from the Experiment in Water in the Temperature Range of (274.05 to 353.05) K

T/K	10 x	T/K	10 x
278.05	0.0796	314.85	0.2615
281.25	0.0932	318.35	0.2910
288.75	0.1191	321.55	0.3214
289.85	0.1281	331.75	0.4028
298.15	0.1704	340.95	0.4767
305.35	0.2030	345.15	0.5261
308.25	0.2126	350.25	0.5854
310.95	0.2332	353.55	0.6459

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Table 2. Mole Fraction Solubility of Taurine Obtained from the Experiment in the Mixture of Water (1) + Methanol (2) in the Temperature Range of (274.05 to 353.05) K[a]

T/K	10 x	T/K	10 x
	$\Phi_2 = 0.05$		
274.35	0.0393	302.85	0.1329
278.15	0.0480	306.55	0.1484
281.55	0.0544	310.25	0.1689
284.65	0.0651	314.15	0.1937
288.35	0.0768	318.15	0.2217
292.75	0.0895	322.45	0.2507
297.15	0.1077	328.65	0.2898
300.75	0.1225	332.45	0.3174
	$\Phi_2 = 0.10$		
276.25	0.0344	308.15	0.1380
280.75	0.0455	310.65	0.1520
284.45	0.0539	315.55	0.1760
287.75	0.0641	317.75	0.1912
291.15	0.0776	320.85	0.2103
297.05	0.0941	324.35	0.2377
301.65	0.1094	328.85	0.2676
305.05	0.1230	331.35	0.2853
	$\Phi_2 = 0.20$		
277.75	0.0234	305.45	0.0874
283.75	0.0301	309.25	0.0987
287.35	0.0359	312.95	0.1142
288.95	0.0394	317.65	0.1388
292.35	0.0462	323.45	0.1691
294.75	0.0540	328.15	0.1923
298.65	0.0656	331.55	0.2104
302.55	0.0773		
	$\Phi_2 = 0.30$		
275.55	0.0131	307.65	0.0685
282.35	0.0209	313.25	0.0864
287.95	0.0283	316.65	0.0990
292.55	0.0342	321.55	0.1202
296.05	0.0403	325.45	0.1374
301.25	0.0490	330.25	0.1572
303.85	0.0564		
	$\Phi_2 = 0.40$		
282.55	0.0124	308.75	0.0426
286.85	0.0178	312.75	0.0517
292.55	0.0223	316.35	0.0609
296.85	0.0271	320.55	0.0731
302.05	0.0326	325.35	0.0870
305.85	0.0369	331.45	0.1028
	$\Phi_2 = 0.50$		
291.15	0.0128	314.65	0.0336
297.05	0.0169	318.75	0.0391
301.65	0.0205	322.55	0.0453
305.25	0.0239	328.15	0.0536
310.35	0.0297	332.25	0.0616

[a] x, mole fraction solubility; Φ_2, volume fractions of methanol in the mixture.

Table 3. Mole Fraction Solubility of Taurine Obtained from the Experiment in the Mixture of Water (1) + Ethanol (2) in the Temperature Range of (274.05 to 353.05) K[a]

T/K	10 x	T/K	10 x
	$\Phi_2 = 0.05$		
277.65	0.0464	302.15	0.1322
281.45	0.0556	307.05	0.1573
285.65	0.0658	310.05	0.1764
288.55	0.0734	314.65	0.2036
291.45	0.0857	318.25	0.2306
295.15	0.1020	323.85	0.2711
298.35	0.1147	328.75	0.3251
	$\Phi_2 = 0.10$		
282.75	0.0551	313.45	0.1703
288.45	0.0720	316.05	0.1829
294.45	0.0904	319.65	0.2001
296.25	0.0993	322.05	0.2149
299.95	0.1082	327.15	0.2460
306.05	0.1274	332.35	0.2799
307.15	0.1355		
	$\Phi_2 = 0.20$		
286.55	0.0491	314.85	0.1549
290.45	0.0576	316.95	0.1689
293.65	0.0687	321.85	0.1957
296.45	0.0797	324.05	0.2099
300.25	0.0962	327.75	0.2337
305.95	0.1121	330.55	0.2549
311.15	0.1397		
	$\Phi_2 = 0.30$		
280.75	0.0294	304.35	0.0804
283.65	0.0343	306.95	0.0913
287.95	0.0419	311.05	0.1091
292.55	0.0477	316.05	0.1297
295.55	0.0556	320.95	0.1496
299.15	0.0633	325.55	0.1700
301.85	0.0708	330.35	0.1959
	$\Phi_2 = 0.40$		
288.55	0.0218	313.15	0.0767
295.25	0.0296	317.55	0.0903
300.05	0.0383	320.05	0.1027
303.35	0.0466	324.15	0.1189
306.05	0.0542	328.95	0.1360
309.05	0.0645	331.15	0.1457
	$\Phi_2 = 0.50$		
288.55	0.0158	316.05	0.0558
292.65	0.0183	319.95	0.0628
297.65	0.0250	323.05	0.0698
302.55	0.0308	325.45	0.0768
308.85	0.0429	331.55	0.0996

[a] x, mole fraction solubility; Φ_2, volume fractions of ethanol in the mixture.

$$\ln\left[1 + \frac{\lambda(1-x)}{x}\right] = \lambda h\left(\frac{1}{T} - \frac{1}{T_m}\right) \tag{3}$$

where A, B, C, A', B', λ, and h are model parameters, x is the mole fraction of the solubility at the system temperature T, and T_m is the melting temperature at the atmospheric pressure.

The experimental points were shown in Tables 1, 2, 3, and 4, and the mole fraction solubility of taurine obtained from the correlation of models was shown in Table SI 1 (SI), where T is the absolute temperature, x is the experimental mole fraction solubility, and x(alp), x(sim), and $x(\lambda h)$ are, respectively, the mole fraction solubility obtained from Apelblat equation, the simplified model of ideal solution, and the λh equation. ARD is the average relative deviation, which is defined as follows:

$$\mathrm{ARD} = \frac{\sum_{i=1}^{n} \frac{x_i(\mathrm{cal}) - x_i}{x_i}}{n} \tag{4}$$

where x(cal) is the mole fraction solubility correlated with the models and x_i is the mole fraction solubility from the experiment.

Moreover, the three models mentioned above were used to correlate the solubility data. All of the parameters of the three models obtained from the correlation are listed in Table 5.

From Tables 1 to 4, Table SI 1 (SI), Figure 1, and Figures SI 2 and SI 3 (SI), it can be found that (1) the solubility of taurine in water + methanol, water + ethanol, and water +

Table 4. Mole Fraction Solubility of Taurine Obtained from the Experiment in the Mixture of Water (1) + 2-Propanol (2) in the Temperature Range of (274.05 to 353.05) K[a]

T/K	10 *x*	*T*/K	10 *x*
	$\Phi_2 = 0.05$		
276.45	0.0459	307.25	0.1579
280.95	0.0558	310.95	0.1788
284.95	0.0664	316.85	0.2202
290.05	0.0852	320.35	0.2425
294.35	0.1000	324.45	0.2719
299.05	0.1186	328.65	0.3010
302.95	0.1352	331.45	0.3239
	$\Phi_2 = 0.10$		
274.75	0.0319	307.15	0.1377
279.95	0.0431	311.75	0.1649
283.65	0.0507	315.95	0.1876
288.55	0.0644	319.95	0.2144
292.75	0.0751	322.55	0.2341
295.35	0.0840	327.35	0.2618
299.35	0.0978	329.55	0.2803
302.85	0.1176		
	$\Phi_2 = 0.20$		
280.75	0.0272	307.75	0.0999
287.35	0.0378	310.85	0.1166
289.95	0.0429	314.85	0.1376
292.65	0.0485	318.15	0.1563
296.45	0.0576	322.45	0.1827
297.65	0.0645	325.25	0.1987
301.65	0.0794	329.75	0.2278
304.25	0.0885		
	$\Phi_2 = 0.30$		
281.15	0.0173	309.55	0.0801
285.25	0.0230	313.15	0.0947
288.95	0.0284	316.15	0.1088
293.05	0.0359	320.15	0.1272
298.15	0.0459	324.25	0.1459
302.65	0.0560	327.95	0.1591
306.05	0.0670	330.45	0.1718
	$\Phi_2 = 0.40$		
283.05	0.0133	308.35	0.0526
287.35	0.0178	311.55	0.0625
293.45	0.0248	314.85	0.0733
299.05	0.0318	319.65	0.0922
302.45	0.0375	323.35	0.1081
305.45	0.0440	328.95	0.1309
	$\Phi_2 = 0.50$		
289.55	0.0163	316.65	0.0518
295.95	0.0213	319.55	0.0590
299.15	0.0243	322.95	0.0666
303.65	0.0309	327.35	0.0762
308.15	0.0381	330.85	0.0844
311.75	0.0427		

[a] *x*, mole fraction solubility; Φ_2, volume fractions of 2-propanol in the mixture.

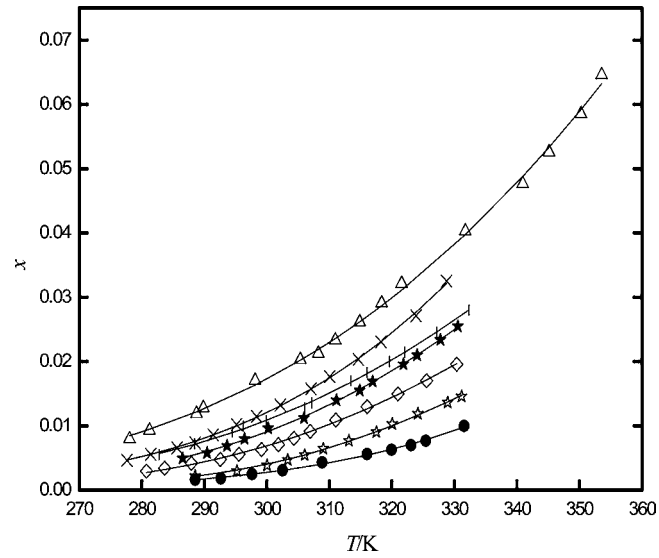

Figure 1. Mole fraction solubility *x* of taurine obtained from the experiment and the correlation of the Apelblat equation in different volume fractions Φ_2 of water (1) + ethanol (2) solution from $T = (274.05$ to $353.05)$ K: △, water; ×, $\Phi_2 = 0.05$; |, $\Phi_2 = 0.10$; ★, $\Phi_2 = 0.20$; ◇, $\Phi_2 = 0.30$; ☆, $\Phi_2 = 0.40$; ●, $\Phi_2 = 0.50$; —, calculated values from the Apelblat equation at corresponding temperatures.

2-propanol solutions with different volume fractions of methanol, ethanol, and 2-propanol (Φ_2), over the temperatures range from (274.05 to 353.05) K, would decrease in following order: 0, 0.05, 0.10, 0.20, 0.30, 0.40, 0.50. It means that the solubility of taurine decreases with the increase of the concentration of methanol, ethanol, and 2-propanol in aqueous solution. (2) The solubility data of taurine in the three solvents mentioned above have the same trend and are closed to each other (Figure 1 and Figures SI 2 and SI 3 of SI). That is to say, methanol and 2-propanol, as a solvent, compared with ethanol, do not have much advantage in the crystallization of taurine. Besides, taking into consideration the cost of production and the security, the water + ethanol solution can be selected as a better solvent for the purification of taurine. (3) The solubility of taurine in water + ethanol solution is low at low temperatures but increases quickly at high temperatures. This characteristic makes the water + ethanol solution available for the recrystallization of taurine. A decrease in temperature and increase in ethanol concentration are beneficial for the crystallization of taurine. (4) From ARD values in Table SI 1 (SI) for the Apelblat equation and the λh equation as well as the simplified model of ideal solution, it can be found that the Apelblat equation was the most accurate of all of these for the systems, and that could be used to correlate the solubility data of taurine in industrial production.

Conclusions

The solubility of taurine can be determined accurately by the laser monitoring technique. The solubility data of taurine in the mixtures of water + methanol, water + ethanol, and water + 2-propanol over the temperature range from (274.05 to 353.05) K increased with increasing temperature and decreased with increasing volume fraction of methanol, ethanol, and 2-propanol in aqueous solution. The Apelblat equation, the simplified model of ideal solution, and the λh equation were used to correlate the solubility data; the three models agreed well with the experimental data. However, the Apelblat equation was the most accurate of all of these for the systems.

Supporting Information Available:

Figure SI 1, comparison of mole fraction solubility *x* from $T = (273.05$ to $354.05)$ K between this work and the literature; Figure SI 2, mole fraction solubility *x* of taurine obtained from the experiment and the correlation of Apelblat equation in different volume fractions Φ_2 of water (1) + methanol (2) solution from $T = (274.05$ to $353.05)$ K; Figure SI 3, mole fraction solubility *x* of taurine obtained from the experiment and the correlation of Apelblat equation in different volume fractions Φ_2 of water (1) + 2-propanol (2) solution from $T = (274.05$ to $353.05)$ K; Table SI 1, mole fraction solubility of taurine

Table 5. Correlation of Model Parameters for Taurine in the Mixture of Water (1) + Methanol, + Ethanol, or + 2-Propanol (2)[a]

		Apelblat equation			simplified model		λh equation	
solvent	Φ_2	A	B/K	C/K^{-1}	A'/K	B'	λ	h/K
water	0	32.00	−3886.06	−4.05	−2569.53	4.51	1.27	2030.24
water (1) + methanol (2)	0.05	120.70	−8401.35	−17.03	−3108.46	5.93	2.18	1441.76
	0.10	85.45	−6928.48	−11.73	−3275.11	6.34	2.50	1325.08
	0.20	214.64	−13255.96	−30.76	−3647.38	7.17	3.04	1210.72
	0.30	158.75	−10916.38	−22.39	−3921.26	7.75	3.40	1162.27
	0.40	92.73	−7901.71	−12.66	−3922.33	7.28	2.08	1893.73
	0.50	90.08	−7535.56	−12.49	−3585.85	5.71	0.73	4889.27
water (1) + ethanol (2)	0.05	51.82	−5456.51	−6.67	−3393.93	6.89	3.63	948.12
	0.10	83.53	−6578.90	−11.59	−2952.03	5.32	1.50	1980.93
	0.20	144.92	−9798.42	−20.51	−3382.05	6.57	2.61	1303.80
	0.30	173.85	−11230.85	−24.79	−3501.48	6.69	2.37	1484.73
	0.40	293.28	−17420.77	−42.20	−4074.40	8.10	3.76	1090.16
	0.50	16.09	−4407.94	−1.28	−4005.67	7.46	2.15	1865.51
water (1) + 2-propanol (2)	0.05	132.06	−8948.97	−18.69	−3133.22	6.04	2.36	1344.15
	0.10	181.98	−11472.79	−26.00	−3405.31	6.78	3.15	1094.78
	0.20	196.62	−12642.53	−27.95	−3914.54	8.12	5.12	772.30
	0.30	289.93	−17097.85	−41.76	−3999.10	8.08	4.18	964.03
	0.40	168.18	−11974.13	−23.48	−4597.40	9.67	7.50	616.97
	0.50	193.37	−12496.17	−27.64	−3779.16	6.67	1.41	2677.00

[a] Φ_2, volume fractions of methanol, ethanol, or 2-propanol in the mixture; A, B, C, A', B', λ, and h are the model parameters.

obtained from the correlation of models in water and the mixture of water (1) + methanol, + ethanol, or + 2-propanol (2) in the temperature range of (274.05 to 353.05) K. This material is available free of charge via the Internet at http://pubs.acs.org.

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