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Original Article

DETERMINATION OF PARTIAL MOLAR PROPERTIES AND ACOUSTIC PARAMETERS OF AMINO ACIDS IN AQUEOUS METHANOL SOLUTIONS IN PRESENCE OF SODIUM BENZOATE

SMRUTI PATTNAIK*, UPENDRA NATH DASH

Institute of Technical Education & Research (SOA), BBSR, Odisha
Email: smrutipattanaik1@gmail.com

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ABSTRACT

Objective: To study the partial molar properties and acoustic parameters of amino acids in the solutions of 5, 10 and 15 wt %of aqueous methanol in presence of sodium benzoate.

Methods: Effect on solute –solvent interaction is studied by determining the densities of pure solvents and the ultrasonic velocity of pure solvent and solutions is measured by using an ultrasonic interoferometer.

Results: The results are discussed in the light of molecular interaction, ion-solvent interactions ion-solvent interactions dominate over ion-ion interactions, β-alanine has higher ion-solvent interaction than α-alanine & glycine.

Conclusion: Overall,β-alanine shows high ion-solvent interaction due to higher mass which represents structural effect of solute on solvent in solution.

Keywords: Amino-acids, Methanol, Ultrasonic velocity, Solvation number, Sodium benzoate.

INTRODUCTION

The study of alcohol– protein interactions is very important for immunology, pharmacology, and medicine. Due to complex molecular structure of proteins direct study is quite difficult. So the amino acids which are the building blocks of proteins are studied. In continuation of our previous work in aqueous medium [1], the present investigation aims at studying the molecular interactions of amino acids in aqueous solutions of (5,10,and15 wt.%) methanol in the presence of 0.1Mcompostion of sodium benzoate ranging from 298.15K to 313.15K at an interval of 5K. Various parameters such as apparent molar volume (V_Φ), limiting apparent molar volume (V^0_Φ), apparent molar expansibility (E_Φ), limiting apparent molar expansibility (E^0_Φ), isentropic compressibility (K_s)and apparent molar compressibility($K_{s,\Phi}$) have been calculated from the density (d) and ultrasonic velocity (U) data, which provide qualitative information regarding molecular interactions

MATERIALS AND METHODS

All the chemicals used were of AnalaR grades and used as such. The solutions of amino acids were prepared on the molal basis and conversion of molality to molarity was done by using the standard expression [3] using the density values of the solutions determined at 298.15K. Conductivity water (Specfic conductance ~10^6 Scm^{-1}) was used to prepare solutions of methanol in presence of 0.1M compostion of sodium benzoate and the solutions were used on the same day. The densities of pure solvents and their solutions were determined by using a specific gravity bottle (25 ml capacity) as described else where [3]. At least 5 observations were taken and differences in any two readings did not exceed ± 0.02%.

The ultrasonic velocity was measured by using Ultrasonic interferometer (Mittal Enterprises, New Delhi, Model No F-81) using a frequency of 2MHz. The precision of the ultrasonic velocity measurement was within ± 0.5 m/s. The amino acids content in the solutions varied over a concentration range of 0.006 to 0.08 mol dm^{-3} in various solvents. Measurement of density was done in the temperature range 298.15K to 313.15K and speed of sound at 298.15K only.

From the density data the apparent molar volume (V_Φ) was calculated by using equation [4]

$$V_\Phi = 1000\,(cd_0)^{-1}(d_0-d) + M_2 d_0^{-1} \quad (1)$$

Where d_0 is the density of solvent

It was found that the V_Φ varied linearly with concentration $c^{1/2}$

The V_Φ data were fitted by a method of least squares to Masson equation [4]

$$V_\Phi = V^0_\Phi + S_v\, c^{1/2} \quad (2)$$

to obtain V^0_Φ (limiting apparent molar volume) and the slope S_E

The apparent molar Expansibility, E_Φ was determined from equation [4]

$$E_\Phi = \alpha_0 V_\Phi + (\alpha-\alpha_0)\,1000c^{-1} \quad (3)$$

The E_Φ data were fitted by a method of least squares to the Masson equation [4]

$$E_\Phi = E^0_\Phi + S_E\, c^{1/2} \quad (4)$$

The ultrasonic velocities 'U' of amino acids in aqueous methanol

Solutions at different concentrations were fitted to an equation of the form [5-7]

$$U = U_0 + Fc + Gc^{3/2} + Hc^2 \quad (5)$$

U_0 is the sound velocity in pure solvent and F,G,H, are the empirical constants

$$U = (K_s d)^{-1/2} \quad (6)$$

The values of K_s obtained were fitted to an equation of the form

$$K_s = K_s^0 + A'c + B'c^{3/2} + C'c \quad (7)$$

where A', B' and C' are the empirical constants.

The apparent molar compressibility $K_{s,\Phi}$ has been computed from equation (8) [5-7]

$$K_{s,\Phi} = 1000\,K_s c^{-1} - K_s^0 d_0^{-1}(1000c^{-1}d - M_2) \quad (8)$$

The $K_{s,\Phi}$ data were fitted to Eqn. 9

$$K_{s,\Phi} = K^0_{s,\Phi} + F'c^{1/2} + G'c \quad (9)$$

to obtain $K^0_{s,\Phi}$ (the limiting apparent isentropic compressibility)

The solvation number S_n can be related to K_s by equation (10)

$S_n = n_1 n_2^{-1}[1-VK_s(n_1 V_1^0 K_s^0)^{-1}]$ (10)

Where V is the volume of the solution containing n_2 moles of solute

V_1^0 is the molar volume of solvent and n_1 is the number of moles of solvent

The variation of solvation number with molar concentration of the solute leads to the limiting solvation number, S_n^0 which was obtained from the relation (11)

$\lim_{c \to 0} K_{s,\varphi} = -S_n^0 V_1^0 K_s^0$ (11)

From the density and sound velocity values,the magnitude of relative association, R_A was calculated from the relation [5-7]

$R_A = (d/d_0)(U_0/U)^{1/3}$ (12)

RESULTS AND DISCUSSION

The values of partial molar volume (V_Φ^0), partial molar expansibility (E_Φ^0), the slope (S_v) of the plot of V_Φ vs $c^{1/2}$ and the slope S_E of E_Φ vs $c^{1/2}$ are given in Table1 for amino acids in different wt.%(5,10, and 15) of methanol in water at temperatures ranging from 298.15K to 313.15K at an interval of 5K.

The density values of the solutions of amino acids vary linearly with concentrations in all wt.% of aqueous solutions of methanol in presence of 0.1 M sodium benzoate at different temperatures. It was found that the V_Φ values vary linearly with $c^{1/2}$ for all the solutions at the experimental temperatures Since V_Φ^0 value indicates the ion-solvent interactions at infinite dilution (as the ion-ion interaction vanishes at infinite dilution), the positive values indicate the presence of ion-solvent interaction which decreases with rise of temperature. The presence of ion-solvent interactions between the molecules promotes structure making effect of amino acids in the solutions of methanol. As observed (Table-1) the V_Φ^0 values of β-alanine are higher in all wt.% of methanol solutions pointing to the fact that ion-solvent interactions take place strongly in β-alanine as compared to the other amino acids solutions. As the magnitude of S_v is a measure of ion-ion interaction, the positive value of S_v, in most of the solutions, are indicative of strong ion-ion interaction. However, they vary with change of temperature and the content of amino acids. As observed magnitudes of V_Φ^0 values are much greater than those of S_v for all the solutions which suggest that the ion-solvent interactions dominate over ion-ion interaction in all the solutions and at all experimental temperatures.

The values of limiting apparent molar expansibility E_Φ^0 (Table 1) are also positive and decrease with increase of temperature, and the values are higher in 15wt.% of methanol solutions than in other wt.%. This may be due to the gradual disappearance of caging or packing effect in the solutions with increase of temperature. But the higher E_Φ^0 values in 15wt.%solutions as compared to those in other wt.% suggest that the appearance of caging or packing effect occurs to a greater extent in the former solution than in the other wt.% of the solutions.

Table 1: Values of V_Φ^0 ($m^3\ mol^{-1}$), S_v($m^{3/2}\ mol^{-3/2}$), E_Φ^0 ($m^3\ mol^{-1}\ K^{-1}$), and S_E($m^{3/2}\ mole^{-3/2}\ K^{-1}$) for amino acids in different wt.%(5,10,and15wt.%) of methanol solutions in presence of sodium benzoate at different temperatures)

Wt%	Temperature (K)	V_Φ^0	S_v	E_Φ^0	S_E
Glycine+methanol+0.1M sodium benzoate					
5	298.15	72.6	8.6	18.7	19.2
	303.15	69.8	8.2	17.8	19.6
	308.15	59.6	84	17.2	19.7
	313.15	56.2	7.8	16.8	196
10	298.15	55.8	6.7	23.8	24.4
	303.15	54.7	5.2	23.6	24.6
	308.15	54.3	4.9	22.8	24.6
	313.15	53.8	9.8	21.6	24.8
	298.15	46.2	9.6	30.9	31.6
15	303.15	45.6	8.8	30.4	31.5
	308.15	45.2	7.9	29.4	31.6
	313.15	44.8	7.2	27.2	31.7

α-Alanine+methanol+0.1M sodium benzoate					
5	298.15	78.4	10.8	30.6	31.4
	303.15	70.6	11.2	30.2	31.5
	308.15	69.2	10.6	29.6	31.6
	313.15	67.4	10.2	29.4	31.6
10	298.15	64.6	9.6	23.4	28.6
	303.15	63.7	8.5	33.6	28.5
	308.15	62.8	6.2	31.2	28.4
	313.15	63.6	6.6	30.6	28.2
15	298.15	58.6	8.6	34.2	26.4
	303.15	57.2	7.7	34.5	26.3
	308.15	53.4	6.4	34.2	26.2
	313.15	52.1	5.6	34.1	26.2
β –alanine+methanol+0.1M sodium benzoate					
5	298.15	90.2	23.6	45.3	46.2
	303.15	89.4	25.2	45.2	46.2
	308.15	87.2	14.6	44.8	46.4
10	313.15	82.4	14.2	44.7	46.4
	298.15	81.9	11.6	46.7	43.1
	303.15	80.2	23.2	46.4	43.6
	308.15	79.4	12.1	46.4	43.1
15	313.15	78.6	12.4	46.3	43.2
	298.15	76.8	23.8	48.8	40.1
	303.15	74.6	24.6	48.4	40.1
	308.15	72.4	24.2	48.3	40.2
	313.15	70.4	24.1	48.1	40.3

A study of ultrasonic behaviour of solutions of in different wt% of aqueous methanol solutions at 298.15K reveals that the sound velocity increases and the isentropic compressibility (K_s) decreases as the contents of methanol in water+.0.1M sodium benzoate increases. The values of U_0 and the empirical constants F, G and H are given in Table 2.

Table 2: Values of U_0 (ms^{-1}) and the constants F, G, H at 298.15K

Wt%	U0(ms-1)	F	G	H
Glycine+methanol+0.1Msodium benzoate				
5	1524.0	1022.4	627.4	-2022.2
10	1536.8	812.2	-1413.2	-1914.6
15	1544.0	413.4	-1028.4	-1128.2
α –alanine+methanol+0.1Msodium benzoate				
5	1552.0	938.2	-1931.0	712.8
10	1564.0	526.2	-1365.2	623.4
15	1572.0	465.4	-1024.6	1816.7
β –alanine+methanol+0.1Msodium benzoate				
5	1524.0	1022.4	627.4	-2022.2
10	1536.8	812.2	-1413.2	-1914.6
15	1544.0	413.4	-1028.4	-1128.2

Such changes are also reported by other workers in other aqueous solvent mixtures like water + methanol [10], and water + PG [11]. As observed, the sound velocity increases with an increase in concentrations of the solutions The values of sound velocities of β-alanine are higher in methanol+.1M sodium benzoate solutions in all wt% than in the solutions of other amino acids. A typical plot of U-U_0/C vs. $C^{1/2}$ in 10wt% of methanol at 298.15K is given in fig1. The value of isentropic compressibility (K_s) decreases with increase in concentration of the solutions in all the amino acids. As observed the values of K_s of β-alanine are less in different wt% of methanol solutions than for other amino acids and are in the reverse order to the sound velocities

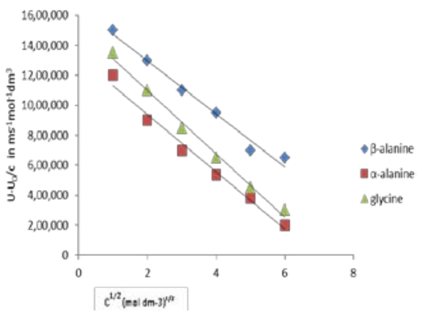

Fig. 1: plot of u-$u_{0//c}$ vs $c^{1/2}$ in 10wt% of methonal solution in presence sodium benzoate

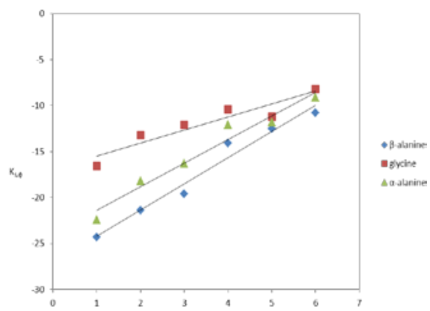

Fig. 2: Plot of $k_{s\varphi}$ vs $c^{1/2}$in 15wt% of methanol solution in the presence of sodium benzoate. The apparent isentropic molar compressibility $K_{s,\Phi}$ increases with concentration of the solutions. The values of $K_{s,\Phi}$ are negative and so also the values of $K^0_{s,\Phi}$. The negative values may be explained by two different phenomena, i. e., electrostriction and hydrophobic solvation. A typical plot of Ks,φ vs $c^{1\backslash 2}$ in 15wt% of methanol +.1sodium benzoate is given in fig2.

The loss of compressibility of the surrounding solvent molecules due to strong electrostrictive forces leads to the electrostrictive solvation. In other words, a tight solvation layer is formed around the ion for which the medium is little compressed by application of pressure.

Table 3: Values of $K^0_{s,\Phi}$ ($m^3\ mol^{-1}\ Pa^{-1}$) and the S^0_n

Wt%	$K^0_{s,\Phi}$	S^0_n
Glycine+methanol+0.1Msodium benzoate		
5	-8.00	-8.00
10	-0.2	-0.2
15	-7.00	-7.00
α- Alanine+methanol+0.1Msodium benzoate	-7.00	
5	-4.00	5.46
10	-0.8	5.48
15	-6.00	5.84
β +Alanine+methanol+0.1Msodium benzoate		
5	-8.00	6.42
10	-6.00	6.48
15	-6.00	6.72

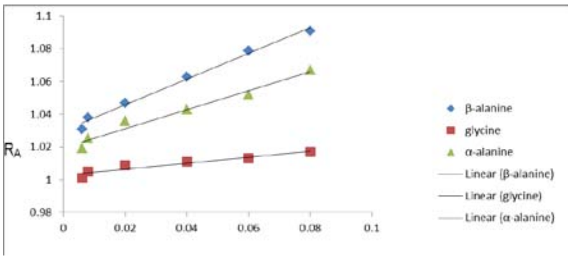

Fig. 3: Plot of R_A vs $c^{1/2}$ acids in 15 wt% of methanol solution in presence of sodium benzoate

The S_n values also increase with increasing methanol content in water higher $S_n^0$for β- alanine in all wt% indicate strong electrostriction as compared to other amino acid solutions.

CONCLUSION

The results of the present investigations on amino acids in aqueous methanol solutions reveal that β-alanine shows high ion solvent interaction in solutions of methanol. The higher sound velocity values of β-alanine in aqueous methanol solutions in presence of sodium benzoate than in other amino acids solutions are due to higher mass. The decrease in value of K_s with increase in wt% of solutions may be due to occupation of the interstitial spaces of water by the solute molecules thereby making the medium less compressible. The increase in R_A values The increase in R_A values with increase in concentration of the solution indicates that ion-solvent interaction dominates over ion-ion interaction in all the solutions. The variation of S_n^0 values predicts the degree of hard electrostrictive solvation, i. e., it represents the structural effect of amino acids on aqueous solutions of methanol in the presence of sodium benzoate.

CONFLICT OF INTERESTS

Declared None

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