

Thermodynamic Studies of Molecular Interactions in Aqueous Glycine-A Biological Molecule

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ABSTRACT: Ultrasonic velocity (u), density (ρ), viscosity (η) were measured for glycine at different concentrations. The experimental data was used to calculate acoustical parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), acoustical impedance (z) and relaxation time (τ). The stability constant (K) was also calculated.

KEYWORDS: Ultrasonic velocity, density, viscosity, molecular interaction, stability constant.

I. INTRODUCTION

On mixing the different solvents the unique behaviour of binary mixtures compared to its constituent counterpart is believed to arise from the nature of the solute solvent interactions. There had been an increased interest in the physicochemical properties of aqueous solutions [1-2]. The nature of the molecular interactions in pure liquids and liquid mixtures can be understood in terms of excess thermodynamic functions [3,4]. Evaluating excess thermodynamic quantities gains more insight into the solution behaviour. Glycine is an organic compound with the formula $\text{NH}_2\text{CH}_2\text{COOH}$. It is the smallest of 20 amino acids. It is a colourless, sweet-tasting crystalline solid. It is used as an additive in pet food and animal feed. For humans, glycine can be used as a sweetener and taste enhancer. Certain food supplements and protein drinks contain glycine. Certain drug formulations include glycine to improve gastric absorption of the drug. Glycine serves as a buffering agent in antacids, analgesics, antiperspirants, cosmetics, and toiletries. The present paper deals with the studies of ultrasonic behaviour of aqueous glycine solution at different concentration. It helps to understand the type and nature of the interactions in the binary mixtures of glycine and water. The amino acid shows lowest solubility in a solution at iso - electric point since there is highest concentration of dipolar ion.

II. EXPERIMENTAL METHOD

AR grade glycine salt is procured. Binary liquid mixtures of glycine with water were prepared of different concentrations (0.01, 0.03, 0.04, 0.06 gm/ml). The density and viscosity of binary mixtures were determined using specific gravity bottle and Ostwald's viscometer respectively. The temperature of this mixtures was maintained at room temperature. The thermodynamic quantities were evaluated using the following expressions.

$$\text{Adiabatic Compressibility } \beta = \frac{1}{\rho u^2} \quad (1)$$

$$\text{Acoustic Impedance } Z = \rho u \quad (2)$$

Relaxation time $\tau = \frac{4\eta}{3\rho u^2}$ (3)

Intermolecular Free length $L_f = \frac{2 \times 10^{-6}}{u\sqrt{\rho}}$ (4)

Internal Pressure $\pi_i = bRT \left(\frac{k\eta}{u} \right)^{\frac{1}{2}} \left(\frac{\rho^{\frac{3}{2}}}{M^{\frac{7}{6}}} \right)$ (5)

Rao's Constant $R = V_m u^{1/3}$ (6)

Wada's Constant $W = V_m \beta^{-1/7}$ (7)

Free volume $V_f =$ (8)

Molecular Association parameter $d = \left(\frac{\rho \eta M u}{M k \eta} \right)^{\left[\frac{3}{2} \right]}$ (9)

Stability constant is found by (ultrasonic method) $K = Y/(b-y)^2$ (10)

The acoustical parameters of aqueous solution of glycine were calculated and shown in Table.1. The stability constant and molecular association parameters of aqueous glycine solution with different concentrations were tabulated in Table.2. and Table.3.

Table.1. Acoustical parameters of glycine

Sample Concentrations g/ml	u ms ⁻¹	ρ Kgm ⁻³	η Nsm ⁻²	$\beta \times 10^{-10}$ Kg ⁻¹ s ⁻² m ⁻¹	$z \times 10^6$ Kgm ⁻² s ⁻¹	$\tau \times 10^{-13}$ secs	$L_f \times 10^{-11}$ m	R	W	$\pi_i \times 10^3$ atmos	V_f (m ³)
0.01	1195.8	1336	0.00147	5.2345	1.5975	9.77	4.57	0.5954	0.0443	22.94	1.8311
0.03	1166.8	1332	0.00114	5.5144	1.5542	8.09	4.69	0.5927	0.0441	23.18	2.534
0.04	1141.2	1329	0.00145	5.7776	1.5164	11.17	4.80	0.5893	0.0438	23.40	1.707
0.06	1133.2	1322	0.00140	5.8463	1.5094	11.30	4.83	0.5869	0.0437	23.53	1.603

Table.2. Determination of stability constant of glycine

Sample Concentrations	u ms ⁻¹	K
0.01	1195.8	4.50
0.03	1166.8	4.52
0.04	1141.2	4.53
0.06	1133.2	4.52

Table.3. Determination of molecular association parameters of glycine

Sample Concentrations g/ml	ρ Kgm ⁻³	η Nsm ⁻²	Association Parameter
0.01	1336	0.00147	26.1
0.03	1332	0.00114	20.2
0.04	1329	0.00145	25.6
0.06	1322	0.00140	24.8

The graphical representation of the variation in free volume and internal pressure with different concentration of aqueous glycine solution were shown in fig.1. and fig.2.

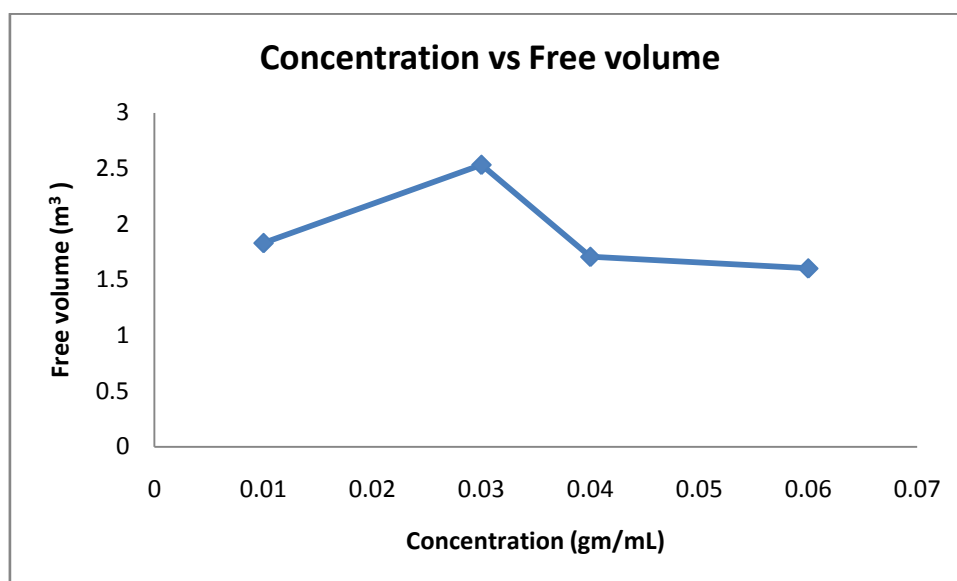


Fig.1. Concentrations vs free volume of glycine

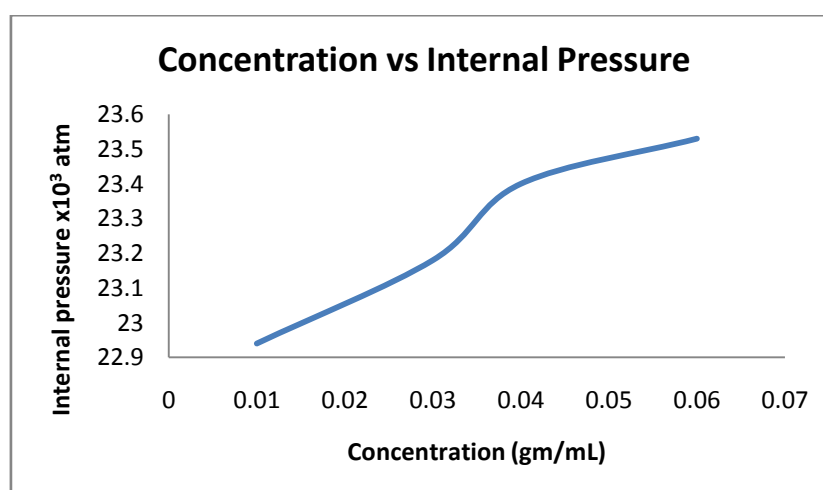


Fig.2. Concentration vs Internal Pressure of glycine

III. RESULTS AND DISCUSSION

It is observed that the value of u ultrasonic velocity decreases gradually as concentration increases. The density value decreases with increase in concentration. Ultrasonic sound velocity in a liquid depends upon the increase or decrease in free length. The compressibility factor is a measure of intermolecular attraction. The compressibility factor shows that there exists an intermolecular attraction between glycine and water. Glycine is a zwitterion which is the only optically inactive amino acid. The addition of biomolecule glycine to water acts as a structure maker. The results is supported by acoustic impedance and compressibility data. The glycine which is a zwitterion causes structural arrangement in the

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neighborhood of water molecule, Decrease in electrostriction increases the compressibility factor. The inter molecular repulsion leads to increase in compressibility factor. The free length signifies weak interaction between glycine and water molecule. Rao's number is positive and is a function of molecular volume and density. The difference in R between successive members of a homologous series is a constant and independent of nature of compounds. Wada's constant is a small number compared with Rao's parameter. It is used to assess the strength of molecular interaction in liquids. The increase in internal pressure is due to the intermolecular repulsion between glycine and water molecule. Free volume is an average volume around which the glycine molecules move. Relaxation time represents the molecular settling time. Stability constant represents positive value. The magnitude of stability constant is positive and small which exhibits weak molecular association between glycine and water. They behave like solutions of substances of high dipole moment. The melting point, solubility, high dipole moment, are consistent with dipolar ion structure, $H_3N^+ - CHH - COO^-$ (Amino acids dipolar ions).

IV. CONCLUSION

Ultrasonic studies reveals hydrogen bonding between glycine and water molecules and addition of glycine increases the solute solvent interaction.

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REFERENCES

- [1] Doty P, "Proteins", Sci American, 1957, Sept pg 173.
- [2] Bohivski RC, et al modern concepts in Bio-Chemistry, 5th edition, Allyn and Bacon. Boston, 1987.
- [3] H Ritzsck and Thomas, W H. Orrville, Molecular interaction, Vols. I, II and III, Wiley Interscience, Newyork, (1989):B.Pullman, Intermolecular Interaction from diatomics to biopolymers, Wiley, Newyork (1978).
- [4] G Barone, G Casstrone, P D Hivecheri and G E Gianithi, J. Chem. Soc. Faraday Trans. I, 85, 207, (1989).