



Role of ultrasonics to study the behaviour of a short peptide in non-aqueous medium

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ABSTRACT

Probing biomolecules by ultrasonic techniques is novel and powerful tool for characterizing their physico-chemical properties. Peptides find wide applications in drug production and as an ingredient in nutritional supplements. Glycyl-L-Glycine is the simplest dipeptide used in biochemical research and in the preparation of biodegradable polymers. Measurement of ultrasonic velocity plays an important role in the study of transport properties of liquids/solution. In the present work, the acoustic and transport properties such as adiabatic compressibility, specific acoustic impedance, intermolecular free length, internal pressure and free volume are computed for various molalities and at various temperatures. The results are analysed on the basis of solute-solvent interactions.

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Introduction

Proteins are of paramount importance for biological systems. All the major structural and functional aspects of the body are carried out by protein molecules [1]. Amino acids and peptides are the fundamental and structural units of proteins. Therefore systematic study of peptides can provide valuable information about the conformational stability of proteins [2]. Amides, the main constituent of proteins and enzymes have attracted the attention of researchers because of their wide biological applications [3,4]. In the present work, formamide is taken as the solvent and interactions of peptides with formamide is analysed on the basis of solute solvent interactions.

Ultrasonics studies of solutions provide knowledge about the molecular interactions, nature and strength of interactions since the ultrasonic velocity is highly sensitive to molecular structure [5-7]. The present study deals with the acoustic and thermodynamic study of glycyl-L-glycine in formamide. The basic parameters such as density, viscosity and ultrasonic velocity are measured for various molalities and at various temperatures, from 5°C to 55°C. From these values, internal pressure (π_i), free volume (V_f), adiabatic compressibility (β), specific acoustic impedance (Z) and intermolecular free length (L_f) are computed.

Materials and method:

Density of the solutions were measured using 25ml specific gravity bottle with accuracy of 0.0001gm/cc. Cannon Fenske viscometer was used for the viscosity measurements, with an accuracy of $\pm 0.5\%$. Mittal's interferometer of frequency 2 MHz with an accuracy ± 0.5 m/s was used for the measurement of ultrasonic velocity.

Formulae used:

1. Internal pressure (π_i) = $bRT [k\eta/u]^{1/2} (\rho^{2/3}/M_{eff}^{7/6})$ atms
2. Free volume (v_f) = $[M_{eff} U/k\eta]^{3/2}$ cc
3. Adiabatic compressibility (β) = $[1/u^2\rho]$ cm²/dyne
4. Intermolecular Free Length (L_f) = $K/(u^2\rho)^{1/2}$
5. Specific acoustic impedance $Z = (\rho u)$ Rayl.

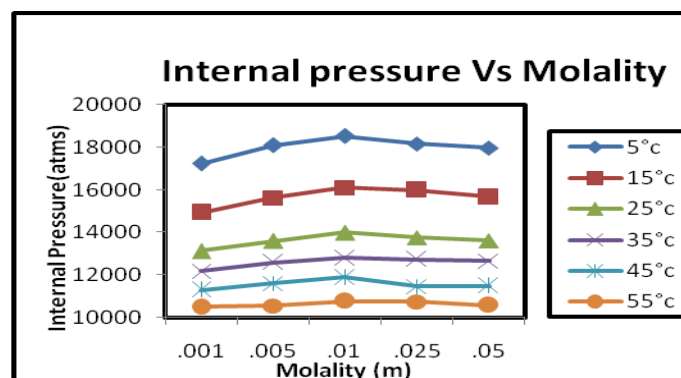
Results and discussions:

Internal Pressure:

Suryanarayana and Venkatesan [8] recognized that the internal pressure of the medium was closely related to the degree of dissociation, ionic mobility, ion pairing, dielectric constant and viscosity. In the present investigation, internal pressure (π_i) increases with increasing molality. At .025 molality, there is a decrease in internal pressure. The decrease in (π_i) with respect to molality suggests that solute-solvent interaction in the system is weak. It is observed that π_i decreases with rise in temperature for all molalities [9,10]. This is because when the temperature is increased, there is a tendency for the ions to move away from each other [11]. Hence there is a reduction in internal pressure with rise in temperature. The results are tabulated in table(1) and shown in fig(1).

Internal pressure-Atmosphere

MOLALITY	5° C	15° C	25° C	35° C	45° C	55° C
.001	17239	14923	13123	12169	11291	10489
.005	18096	15635	13586	12587	11602	10559
.01	18519	16105	13988	12787	11881	10767
.025	18167	15993	13763	12737	11455	10739
.05	17971	15663	13613	12657	11483	10571



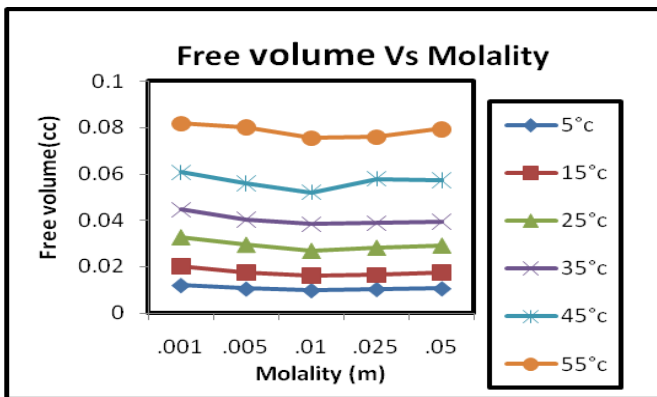
Free Volume:

Free volume is one of the significant factors in explaining the variations of the physico-chemical properties of liquids and

solutions. The observed values of free volume (V_f) for various molalities and temperatures are tabulated in table (2) and shown in fig(2). The free volume increases with increasing temperature and decreases with increasing concentration upto .01m. The decrease in (V_f) indicated that there is a close packing of molecules with increase in solute concentration[12]. The sudden increase in (V_f) therefore confirms the weak solute-solvent interaction.

Free Volume (CC)

MOLALITY	5° C	15° C	25° C	35° C	45° C	55° C
.001	0.0120	0.0203	0.0326	0.0446	0.0607	0.0817
.005	0.0104	0.0177	0.0294	0.0402	0.0559	0.0802
.01	0.0097	0.0162	0.0268	0.0384	0.0521	0.0755
.025	0.0102	0.0165	0.0282	0.0387	0.0579	0.0759
.05	0.0105	0.0175	0.0291	0.0394	0.0573	0.0794

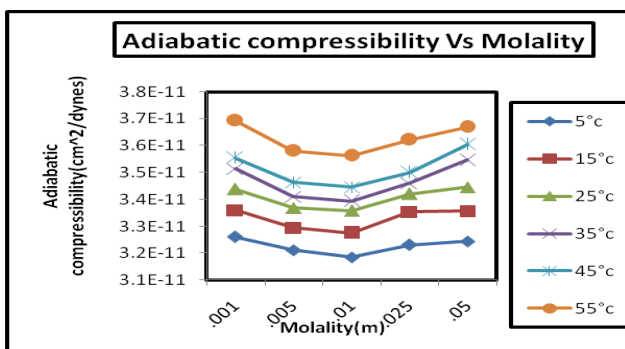


Adiabatic compressibility(β) :

Intramolecular and intermolecular association, complex formation and related structural changes affect the compressibility of the system which in turn produces corresponding variations in the ultrasonic velocity[13]. It is known that amino acid molecules in neutral solution exist in dipolar form and have interaction with the surrounding molecules. In the present investigation, β decreases with increase in molality. This confirms the presence of solute-solvent interaction through dipole-dipole interaction of the -OH group of peptides with surrounding formamidemolecules[14]. The results are tabulated in table (3) and shown in fig (3).

Adiabatic Compressibility-cm²/dyne

Molality	5° C	15° C	25° C	35° C	45° C	55° C
.001	3.261E-11	3.359E-11	3.438E-11	3.514E-11	3.553E-11	3.692E-11
.005	3.212E-11	3.295E-11	3.368E-11	3.410E-11	3.464E-11	3.580E-11
.01	3.186E-11	3.275E-11	3.358E-11	3.393E-11	3.446E-11	3.563E-11
.025	3.230E-11	3.354E-11	3.420E-11	3.461E-11	3.500E-11	3.622E-11
.05	3.245E-11	3.357E-11	3.445E-11	3.546E-11	3.604E-11	3.669E-11

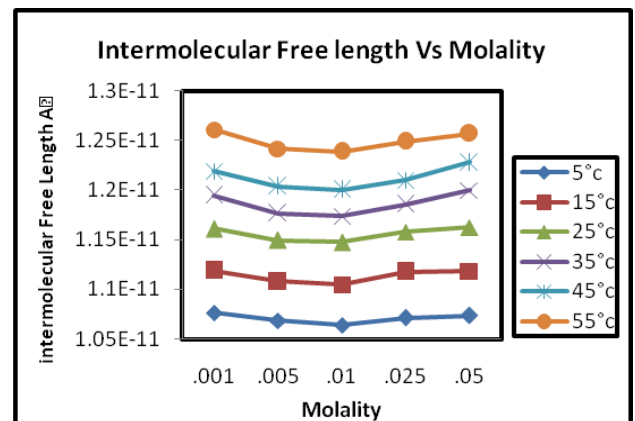


Intermolecular frelength(L_f) :

The intermolecular frelength is one of the important acoustical paramters in determining the nature of the interaction between the components of the solution. The results of variations of intermolecular frelength for various concentrations and temperatures are tabulated in table(4) and shown in fig(4). The non linear variations observed in intermolecular frelength indicates the dissociation of ions taking place in solutions. The decreased compressibility brings the molecules to a closer packing resulting in a decrease in the intermolecular frelength[15].

Inter-Molecular Free Length-A°

Molality	5° C	15° C	25° C	35° C	45° C	55° C
.001	1.076E-11	1.119E-11	1.161E-11	1.195E-11	1.219E-11	1.261E-11
.005	1.068E-11	1.108E-11	1.149E-11	1.177E-11	1.204E-11	1.241E-11
.01	1.064E-11	1.105E-11	1.147E-11	1.174E-11	1.201E-11	1.239E-11
.025	1.071E-11	1.118E-11	1.158E-11	1.185E-11	1.210E-11	1.249E-11
.05	1.074E-11	1.118E-11	1.162E-11	1.200E-11	1.228E-11	1.257E-11



Specific Acoustic Impedance(z):

The acoustic impedance is the paramter related to the elastic properties of the medium. Therefore it is important to examine the acoustic impedance in relation to the concentration and temperature. The observation of Z with respect to molality and temperature are tabulated in table(5) and shown in fig(5). In the present analysis, it is found that Z decreases with rise in temperature and increases with increasing molality. An abrupt change is accounted at .025m which may be due to weak solute-solvent interactions.

Specific Acoustic Impedance(RAYL)

SP-AC-IMPEDANCE	5° C	15° C	25° C	35° C	45° C	55° C
.001	18.730	18.398	18.135	17.875	17.724	17.317
.005	18.891	18.598	18.327	18.146	17.955	17.592
.01	18.970	18.663	18.338	18.192	18.002	17.631
.025	18.831	18.439	18.182	18.015	17.856	17.486
.05	18.792	18.432	18.133	17.805	17.607	17.381

Conclusion:

A systematic acoustical study of glycy glycine with formamide has been carried out at different concentrations and temperatures. The applications of peptides show that they play a vital role in our life being involved in various biological processes and also have medicinal uses. Formamide, an important biological solvent is the simplest compound contains

-CO -NH- fragments which is present in peptides and proteins. The various parameters computed in the present investigation, provide valuable information and helps us to explore the applications of glycyl-L-glycine for medicinal and pharmaceutical purposes.

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