

Analysis of Transport Properties of Some Glycyl Peptides in Non-Aqueous Medium

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Abstract: *The thermodynamical parameters of three glycyl dipeptides have been analysed in non-aqueous medium of formamide at various molalities and temperatures. Peptides play a vital role in the field of medicine and Pharmaceutical industries. Peptides have been used in the study of protein structure and function. They are used in nutritional supplements. In view of their use, the study of structural changes due to transport properties gives an impetus and interest in the field of liquid state. The main advantage of considering the internal pressure in calculating the transport properties lies in the fact that it is experimentally measurable, and it depends on molar volume. In the present work, density, viscosity and ultrasonic velocity of Glycyl -L-Leucine, Glycyl -L-Valine and diglycine were measured in the temperature range of 5°C to 55°C. From the above values internal pressure, free volume were calculated. The results are analysed based on peptide amide interactions.*

Keywords: peptides, internal pressure, free volume, ion-solvent interactions.

1. Introduction

Measurement of ultrasonic velocity plays an important role in the study of transport properties of liquids / solutions. Acoustic and thermodynamic properties have been used to understand various types of intermolecular interactions and provide qualitative information about the physical nature and strength of the molecular / inter-ionic interactions. The ultrasonic velocity data combined with density and viscosity provide the standard means for determining the internal pressure, free volume and various acoustical parameters.

Internal pressure (π_i) and free volume (V_f) are the thermodynamical parameters, which are useful in understanding the intra and inter molecular interactions. It is known that the solute is made up of charged particles, and hence there is resultant inter-ionic interactions and the internal pressure of the medium that modulates the electrical conductance of a solution. Free volume is one of the most significant parameters in explaining the variations in the physico-chemical properties of liquids.

Peptides have attracted much attention as potential drugs due to their high selectivity, efficient activity and low toxicity [1-2]. Dipeptides are the simplest molecules which are the building blocks of other more complex biomolecules such as proteins and peptides. Thus they can be used as model compounds for the study of the behavior of complex biomolecules [3-5]. Glycyl -L-Valine peptide acts as a nutritional supplement and pharmaceutical intermediate. Glycyl-L-Glycine is the simplest dipeptide used in biochemical research and in the preparation of biodegradable polymers.

Amides, the main constituent of proteins and enzymes have attracted the attention of researchers because of their wide biological applications [6]. The solution structure is of great importance in understanding the nature of bioactive molecules in the body. [7-8] Ultrasonic studies of solutions

yield valuable information about the molecular interactions, nature and strength of interactions since the ultrasonic velocity is highly sensitive to molecular interactions [9-11]. The velocity of ultrasonic waves in a medium and several other acoustical parameters which are dependent on it help to determine the overall response of the medium. In the present work, non-aqueous solutions of Glycyl peptides have been prepared with different concentrations and the experiments were carried out from a low temperature of 5°C to a high temperature of 55°C.

2. Experimental Technique

Density of the solutions is measured using 25ml specific gravity bottle with an accuracy of 0.0001 gm/cc. Cannon Fenske viscometer is 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 is used for the measurement of ultrasonic velocity.

COMPUTATION

Internal pressure (π_i) and free volume (v_f) are evaluated by using the following formulae.

$$(i) \text{ Internal pressure } (\pi_i) = bRT [k\eta / u]^{1/2} [\rho^{2/3} / M^{7/6}] \text{atms}$$

$$(ii) \text{ Free volume } (v_f) = [M_{\text{eff}} u / k\eta]^{3/2} \text{cc}$$

Table 1: GLYCYL -L-GLYCINE Internal pressure(atms)

Molality	5°C	15°C	25°C	35°C	45°C	55°C
.001	17239	14923	13123	12169	11290	10489
.005	18096	15635	13586	12587	11601	10558
.01	18519	16105	13987	12787	11881	10766
.025	18167	15992	13763	12736	11455	10739
.05	17971	15663	13613	12657	11483	10570

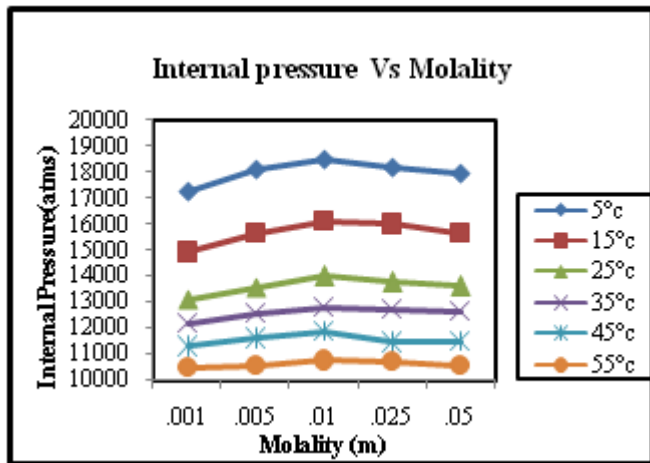


Figure 1
GLYCYL -L-GLYCINE

Table 2: FREE VOLUME (cc)

Molality	5°C	15°C	25°C	35°C	45°C	55°C
.001	0.012	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
.015	0.0102	0.0165	0.0282	0.0387	0.0579	0.0759
.02	0.0105	0.0175	0.0291	0.0394	0.0573	0.0794

GLYCYL -L-GLYCINE

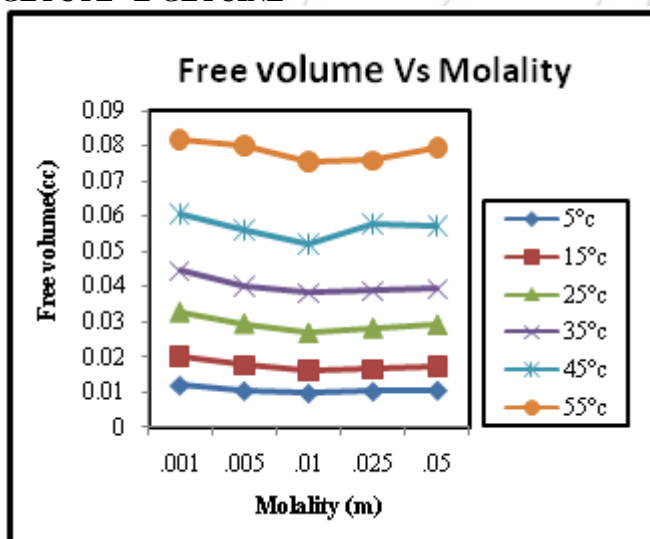


Figure 2: GLYCYL- L -LEUCINE

Table 3: Internal pressure(atms)

Molality	5°C	15°C	25°C	35°C	45°C	55°C
.001	20180	17725	14433	13006	11976	11017
.005	18869	16585	14136	12914	11850	10792
.01	19859	16748	14608	13099	12124	10805
.015	18619	16230	13939	12870	11909	10714
.02	18924	15588	13683	12513	11656	10544

GLYCYL- L- LEUCINE

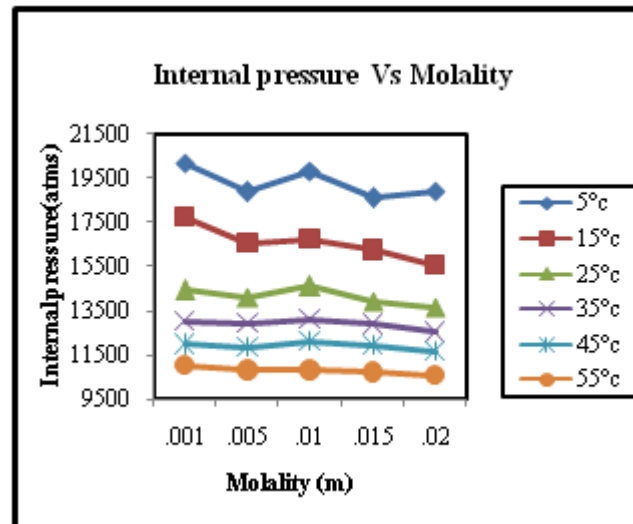


Figure 3:

GLYCYL- L- LEUCINE

Table 4: FREE VOLUME(cc)

Molality	5°C	15°C	25°C	35°C	45°C	55°C
0.001	0.0075	0.0123	0.0247	0.0366	0.0510	0.0709
0.005	0.0092	0.0149	0.0263	0.0373	0.0526	0.0753
0.01	0.0079	0.0144	0.0238	0.0358	0.0491	0.0752
0.015	0.0095	0.0159	0.0273	0.0376	0.0517	0.0769
0.02	0.0091	0.0178	0.0288	0.0410	0.0551	0.0807

GLYCYL -L- LEUCINE

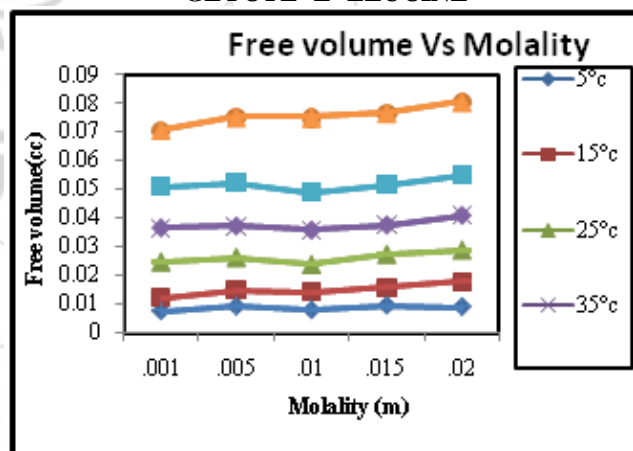


Figure 4:

GLYCYL -L- VALINE

Table 5: Internal pressure(atms)

Molality	5°C	15°C	25°C	35°C	45°C	55°C
.001	18557	15127	13118	12939	10932	10554
.005	19666	16403	14015	13586	12236	10880
.01	19648	16301	14017	13531	12066	10719
.015	19654	16328	13727	13236	12057	10627
.02	20028	16172	13735	13103	11954	10611

GLYCYL -L- VALINE

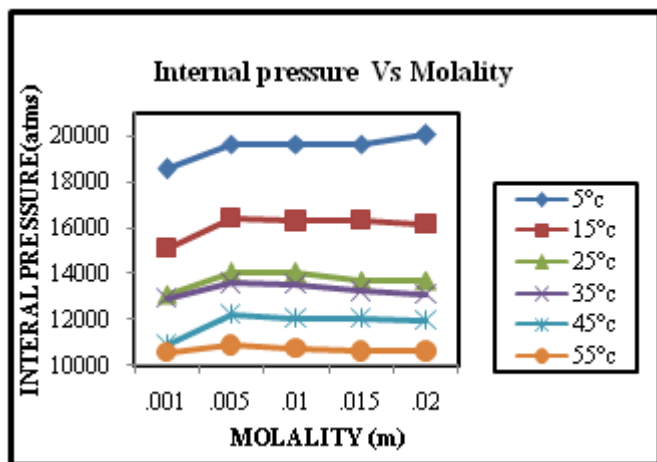


Figure 5:

GLYCYL- L -VALINE

Table 6: FREE VOLUME(CC)

Molality	5°C	15°C	25°C	35°C	45°C	55°C
0.001	0.0096	0.0197	0.0328	0.0372	0.0670	0.0808
0.005	0.0081	0.0154	0.0269	0.0320	0.0478	0.0736
0.01	0.0081	0.0156	0.0269	0.0325	0.0498	0.0771
0.015	0.0081	0.0156	0.0286	0.0346	0.0499	0.0789
0.02	0.0076	0.0160	0.0285	0.0357	0.0511	0.0794

GLYCYL- L -VALINE

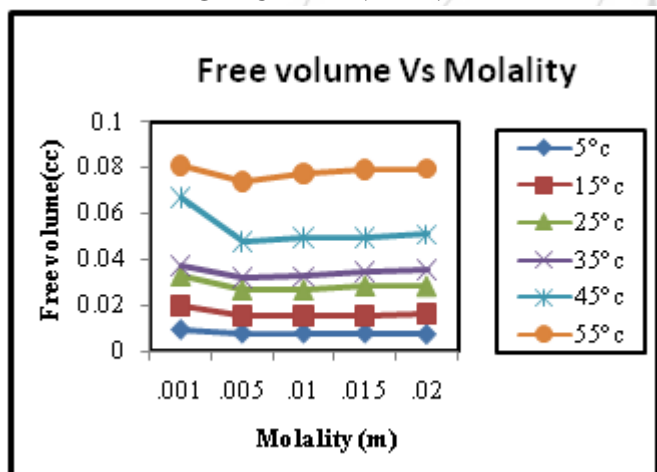


Figure 6

3. Result And Discussion

Internal pressure of a solution is a single factor which appears to vary with intermolecular interactions namely, solvation, quantum mechanical forces of dispersion, dielectric forces. The solute-solvent interaction which plays an important role in the study of transport properties of solutions. The interaction depends upon the solvent and solute structure and presence of temperature.

In the present investigation, the internal pressure exhibits an increasing trend with respect to increasing molalities, in short peptide Glycyl-L-Valine as shown in fig (5). The variations indicate, that there is a strong solute-solvent interaction between the solute and solvent. The cohesive energy is enhanced, which is due to *zwitterionic nature of a peptide* ($-NH_2$ group is a base, $-CO_2H$ group is an acid.) H^+ ion is therefore transferred from one end of the molecules to the other end of the molecule, to form a zwitterion[12].

This behaviour may be attributed to structure making nature of the solute in the solvent[13]. In Glycyl-L-Leucine, the internal pressure is found to decrease at 0.005m, as shown in fig (3) and in Glycyl-L-Glycine from 0.025m, as in fig (1) at all the temperatures.

This decrease in internal pressure supports the weak ion-solvent interaction. The decreasing trend in internal pressure reveals the tendency of the breaking structure breaking nature of the solvent[14]. Free volume is one of the significant factors in explaining the variations in the physico-chemical properties of liquids, solution and the liquid mixtures. The free space and its dependent properties have close connection with molecular structure. Free volume is the effective volume in which a particular molecule can move. The free volume decreases with respect to concentration as expected. The structure making and breaking effect are also confirmed by the decreasing and increasing the value of free volume with respect to molalities and temperature. The variations of free volume with respect to molalities and temperatures are also confirm that there is a strong solute-solvent interaction in Glycyl-L-Valine heteropeptide solutions[15].

4. Conclusion

In the present work a detailed thermodynamic analysis of three peptides was made. The study reveals the existence of a strong solute-solvent interaction in Glycyl - L-Valine, structural stabilization in Glycyl- L- Glycine and weak ion-solvent interaction in Glycyl -L- Leucine. Zwitterionic behavior is identified in Glycyl- L- Valine and peptide-amide interaction is envisaged.

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