

# Prediction of Internal Pressure and Surface Tension and their Correlation with Molecular Interaction in Aqueous Amino Acids

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**Abstract:** *Ultrasonic velocity, density and viscosity were measured in six aqueous amino acids namely L-Alanine, L-Aspartic acids, L-Glutamic acid, L-Glutamine, L-Phenylalanine and L-Valine of different concentration at 303.15K. Attempts have been made to show the significance of thermodynamics properties like internal pressure and surface tension with molecular interaction in aqueous amino acids. The internal pressure and surface tension were evaluated using experimentally determined ultrasonic velocity, density and viscosity.*

**Keywords:** ultrasonic velocity, internal pressure, surface tension, density, viscosity, amino acids

## 1. Introduction

The significance of the internal pressure and its correlation with the solubility parameter (widely used for instance in paints, pharmaceuticals, polymers, and petroleum industry) has been discussed among others in review articles by Barton<sup>[1]</sup> and Deck<sup>[2]</sup>.

The same problem in relation to the pressure influence was investigated by Renuncio et al.<sup>[3]</sup> and recently by Verdier and Andersen<sup>[4]</sup>. Internal pressure is a measure of how the internal energy of a system changes when it expands or contracts at constant temperature. The most significant effect of the increase in pressure is the decrease in volume, i.e., a decrease in the molecular distance and free volume. This leads to variation of the molecular interactions. It is known that the internal pressure can be expressed as sum of an attractive and repulsive contribution. The attractive contributions are connected with the attractive forces that mainly comprise hydrogen bonding, dipole-dipole, multipolar, and dispersion interactions. Repulsive forces, acting over very small intermolecular distances, play a minor role in the cohesion process under normal conditions. But as the pressure increases, the repulsive forces increase also. At the same time change in the attractive forces are more complicated. In consequence, the internal pressure can both increase and decrease, as well as reaches a maximum as the pressure increases. And in some cases, the internal pressure can be even insensitive to pressure. Compression causes decrease in  $P_{int}$  that it becomes highly negative. In other words, the decrease in the molecular distance causes that the repulsive forces completely dominate the attractive forces. Because molar volumes reflect changes in the molecular distance (as a pressure is applied or as the liquid contract on cooling), Barton<sup>[5]</sup> has discussed the relationship between  $P_{int}$  and molar volumes.

Surface tension and surface energy balanced with the internal pressure. Surface effects (surface energy) play critical role many kinetics process of materials, such as the particle ripening and nucleation. Essentially every phase transformation begins with the formation of a tiny spherical particle called nucleus. The surface/interface separating the two, the particle and the matrix, is characterized by the existence of surface energy. It is thus necessary to account for the existence of the surface when defining thermodynamic quantities.

The physical and chemical behavior of liquids cannot be understood without taking surface tension into account. It governs the shape that small masses of liquid can assume and the degree of contact a liquid can make with another substance. Surface tension is caused by the attraction between the molecules of the liquid by various intermolecular forces. In the bulk of the liquid each molecule is pulled equally in all directions by neighboring liquid molecules, resulting in a net force of zero. At the surface of the liquid, the molecules are pulled inwards by other molecules deeper inside the liquid and are not attracted as intensely by the molecules in the neighboring medium (e.g., vacuum, air or another liquid). Therefore all of the molecules at the surface are subject to an inward force of molecular attraction which can be balanced only by the resistance of the liquid to compression.

Ultrasonic has become an important and widely accepted method to study the thermodynamic properties of liquid system. Thus characterization of the materials by the determination of Ultrasonic wave propagation parameters is encouraged. In the present communication the internal pressure and surface tension were evaluated using experimentally determined ultrasonic velocity, density and viscosity and further the concept of these parameters has used to study the molecular interaction in aqueous amino acids.

## 2.Theoretical

Internal pressure is defined as a partial derivative of internal energy with respect to volume at constant temperature: Thermodynamically, the internal pressure can be calculated using the formula as

$$P_{int} = bRT^3 \left[ \left[ \frac{K_j \eta}{u} \right]^{1/2} \left[ \frac{\rho^{2/3}}{M^{1/6}} \right] \right] \quad N/m^2 \quad \text{----(1)}$$

Where

$P_{int}$  =Internal Pressure,  $b$ = Vander Waal's constant,  $R$ = Gas constant= 8.314 J/K mol

$T$ = Temperature in Kelvin,  $K_j$ = Jacobson's constant = 4.2 x10<sup>-9</sup>,  $\eta$ = Viscosity

$u$ = ultrasonic velocity,  $\rho$ = density,  $M$ =Molecular weight

and the surface tension is measured by Young-Laplace equation

$$S_{\Gamma} = P_{int} r/2 \quad N/m \quad \text{-----(2)}$$

Where

$S_{\Gamma}$  = surface tension,  $P_{int}$ = internal pressure,  $r$ = molecular radius

## 3. Materials and Methods

All the given sample L-Alanine, L-Aspartic acids, L- Glutamic acid, L- Glutamine, L- Phenylalanine and L- Valine were in pure form (E –Merck grade). Different concentration (0.0075M, 0.008M, 0.0085M, 0.009M, 0.0095M, 0.01M) of each sample were made with doubled distilled water. Ultrasonic velocities were experimentally determined with Pulse Echo Overlap Method using Innovative Instrument-102 interferometer along with ultrasonometer (4MHz) and Universal time & frequency counter. Densities were determined with Density Bottle with plunger method and viscosity with Ostwald's viscometer.

## 4. Results

The liquid system taken for the present investigation were L- Alanine, L-Aspartic Acid, L-Glutamic Acid, L-Glutamine, L-Phenylalanine and L-Valine in water having conc. 0.0075M, 0.008M, 0.0085M, 0.009M, 0.0095M, and 0.01M. Fig (1),(2), (3) ,(4) and (5) showing respectively the variation of ultrasonic velocity( $u$ ), density( $\rho$ ), viscosity( $\eta$ ), internal pressure ( $P_{int}$ ) and surface tension ( $S_{\Gamma}$ ) with different concentration of L-Alanine, L-Aspartic Acid, L- Glutamic Acid, L-Glutamine, L-Phenylalanine and L-Valine in water at 303.15K

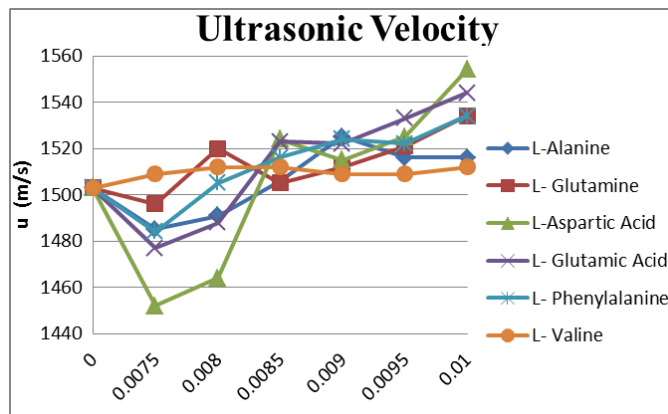


Figure 1

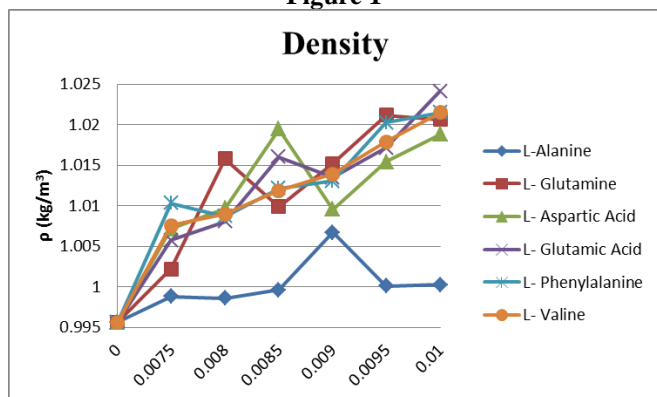


Figure 2

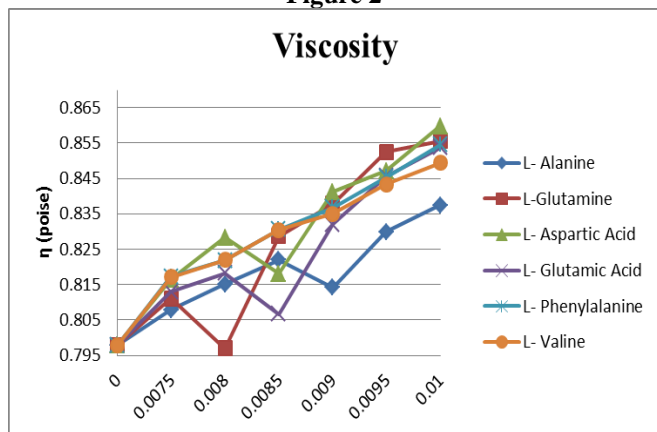


Figure 3

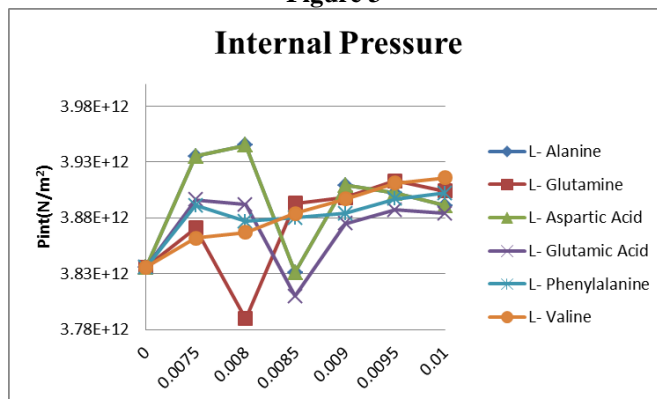


Figure 4

## 5. Discussion

From the above figs it was observed that ultrasonic velocity ( $u$ ) increases with concentration. This is due to breaking of cluster of water molecule by the amino acid molecule

resulting in enhancing the closed packed structure of water (association). The graph of density ( $\rho$ ) supports the association. The factor apparently responsible for such behavior may be the presence of interaction caused by the proton transfer reaction of amino acid and hydrophilic nature of solution. The increase in association may be due to water enhancement brought by the increase in electrostriction. The electrostriction effect which causes shrinkage in the volume of solvent is caused by zwitterionic portion of the amino acids. The increase in ultrasonic velocity and density supports this interaction. Amino acid molecules in the neutral solution exist in dipolar form and they have stronger interaction with surrounding water molecules. The increasing electrostrictive compression of water around the molecule results in a larger increase in the density of associated molecule formed in the solution.

Internal pressure ( $P_{int}$ ) is one the significance thermodynamic property of any system which can be used to study the molecular interaction in a given system. The increase in internal pressure with molar concentration may be due to increasing strength of dipolar association or formation of hydrogen bonding or complex formation between the component molecules while the decrease in internal pressure with molar concentration may be due to weakening of dipolar association or breaking up of hydrogen bonding. Internal pressure is a measure of how the internal energy of a system changes when it expands or contracts at constant temperature. The most significant effect of the increase in pressure is the decrease in volume, i.e., a decrease in the molecular distance and free volume. This leads to variation of the molecular interactions. The decrease in volume increases the density of associated molecule formed in the solution. The increase in viscosity with molar concentration supports the above fact of increasing the association nature of solute with water molecule.

From the above fig. it was observed that the internal pressure showing increasing trend for all given sample which shows that dipole-dipole interaction or H-bonding is predominated in aqueous amino acids. The values of ultrasonic velocities, densities and viscosities also support the result. The irregular increasing trend only shows that at certain concentration the association (or H-Bonding) is more or that concentration is favorable for molecular association. This hydrophilic interaction gives the solvent related force and associating nature of both solvents and solution.

The surface tension ( $S_T$ ) shows the opposite trend to that of increasing internal pressure. This decreasing nature of surface tension with molar concentration shows the increasing molecular radius of the formation of composite molecule and hence the association nature of both solute and solvent. Surface tension is a contractive tendency of the surface of a liquid that allows it to resist an external force. The cohesive forces among liquid molecules are responsible for the phenomenon of surface tension. In the bulk of the liquid, each molecule is pulled equally in every direction by neighboring liquid molecules, resulting in a net force of zero. The molecules at the surface do not have other molecules on all sides of them and therefore are pulled inwards. This creates some internal pressure and forces liquid surfaces to contract to the minimal area. This study

should be applicable to characterize the mechanical properties of various cellular systems.

## 6. Conclusion

All the above discussion shows that there will be molecular association (or dipole- dipole interaction or dipole-induced dipole interaction) when we add amino acids to pure water. This shows that molecular interaction occur in aqueous amino acids. Hence internal pressure and surface tension are can be used to study the molecular interaction in a given system and this study should be applicable to characterize the mechanical properties of various cellular systems.

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