

STUDY OF MOLECULAR INTERACTION THROUGH FREE VOLUME AND INTERNAL PRESSURE OF AQUEOUS AMINO ACIDS

AT. Shende^{1*}, PV. Tabhane² and VA. Tabhane³

¹Department of Physics, Institute of Science, Nagpur, Maharashtra, India.

²Department of Physics, R.T.M. Nagpur University, Nagpur, Maharashtra, India. ³Department of Physics, University of Pune, Ganeshkhind, Pune, Maharashtra, India.

ABSTRACT

Ultrasonic Velocity, Density and Viscosity were measured in six aqueous amino acids namely; L-Alanine, L-Aspartic Acid, L-Glutamic Acid, L-Glutamine, L-Phenylalanine and L-Valine of different concentration at 303.15 K. Free volume and internal pressure were evaluated using experimentally determined ultrasonic velocity, density and viscosity. The free volume and internal pressure were used to study molecular interaction in aqueous amino acids.

Keywords: Free volume, internal pressure, ultrasonic velocity, density, viscosity.

1. INTRODUCTION

Internal pressure is the resultant of attractive and repulsive forces between the molecules. It measures the molecular cohesion and instantaneous volume derivative of the cohesive energy associated with an isothermal expansion of liquid. The internal pressure of hydrogen bonded liquids (water) is large as compared to non-hydrogen bonded liquid. Hence internal pressure in solution can be used for studying the molecular association through hydrogen bonding. Free Volume and Internal pressure, a fundamental properties of the liquid state has been studied initially by Hildebrand *et al*^{1,2} and subsequently by several workers³⁻⁹. The importance of internal pressure in understanding condensed matter has been established by several workers. The study of thermodynamic and transport properties of liquid system has gained much importance during recent years¹³ the molecular interaction in liquid solution can be study by free volume and internal pressure. For this, we have experimentally determined simultaneously the density, viscosity and

ultrasonic velocity of given aqueous amino acids.

2. THEORETICAL

The free volume can be computed at any temperature using the following formula

$$V_f = (V/u^3)(\gamma RT/M)^{3/2} \dots \dots \dots (1)$$

Where V is molar volume, u is ultrasonic velocity, γ is adiabatic constant having value 1.4, R is molar gas constant having value 8.314 J/mol-K, T is temperature and M is molecular weight

In a series of papers, Suryanarayan *et al*⁴ used a method for computing the internal pressure of a liquid from its density, viscosity and ultrasonic velocity. They obtained the following expressions for the internal pressure on the basis of dimensional analysis using free volume concept.

$$P_{int} = bRT (k \eta / u)^{1/2} \rho^{2/3} / M^{7/6} \dots \dots \dots (2)$$

Where b is packing factor, k is a constant independent of temperature having a value of 4.28×10^9 and η is the viscosity. The other symbols have their usual meaning. Thus (2) affords a method for estimating P_{int} from a knowledge of η , ρ and u .

3. MATERIALS AND METHODS

All the given sample L-Alanine, L-Aspartic Acid, 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. Densities, Viscosities and ultrasonic velocities were measured at 303.15 K. Densities were determined with Density Bottle with plunger method. Viscosities were determined with Oswald Viscometer and Ultrasonic Velocities with Pulse Echo Overlap Method using Innovative Instrument-102 (AUAR) along with Ultrasonometer (4 MHz) and Universal Time & Frequency Counter.

4. RESULT

The liquid system taken for the present investigation were L-Alanine, L-Aspartic Acid, L-Glutamic Acid, L-Glutamine, L-Phenylalanine and L-Valine having conc. 0.0075M, 0.008M, 0.0085M, 0.009M, 0.0095M, and 0.01M. Experimentally values of Densities, Viscosities and Ultrasonic velocities with different concentration at 303.15K were calculated

Free volume and internal pressure values for all pure liquid system were calculated from Equ. (1) and (2).

Fig (1),(2), (3), (4) (5) and (6) showing respectively the variation of Free Volume (V_f) and Internal Pressure (P_{int}) with different concentration of L-Alanine, L-Aspartic Acid, L-Glutamic Acid, L-Glutamine, L-Phenylalanine and L-Valine at 303.15K

5. DISCUSSION

Internal pressure plays an important role in explaining molecular interaction, as this represents the resultant of the forces of attraction and repulsion between the molecules. As observed, internal pressure (P_i) increases with concentration. The free volume (V_f) is found to decrease with concentration. Both P_i and V_f show irregular change with increase of chain length of amino acids. Ion solvent interaction is affected by two factors: (i) the breaking up of the solvent structure on addition of solute to it and (ii) the solvation of solute. At any point, the interaction as observed is the resultant of the two factors. The decrease of V_f (increase of P_i) indicates the formation of hard or tight solvation layer around the ion and increase of V_f (decrease of P_i) may be due formation of thin or loose solvation layer. As observed solvation layer formed around given amino acids complex is hard or tight. This may be due to fact that the given amino acids experience an additional hydrophobic hydration. The increasing tendency indicates the presence of some specific interaction which may be due to dipole-induced dipole interaction between unlike molecules in the components.

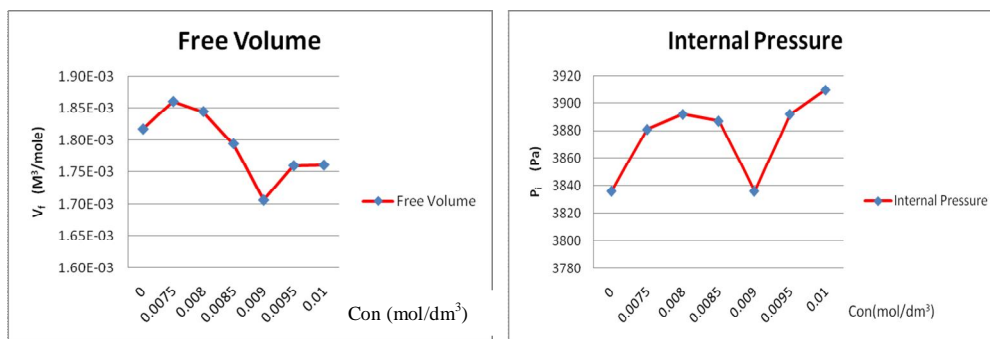


Fig. 1: Free Volume and Internal Pressure for aqueous L-Alanine at 303.15K

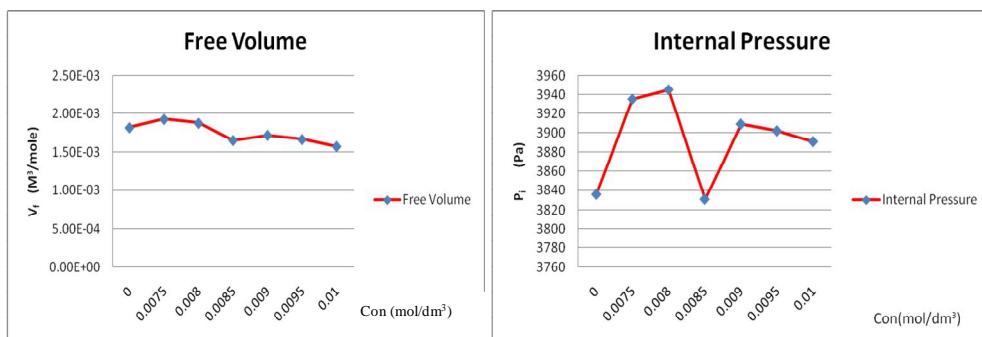


Fig. 2: Free Volume and Internal Pressure for aqueous L-Aspartic Acid at 303.15 K

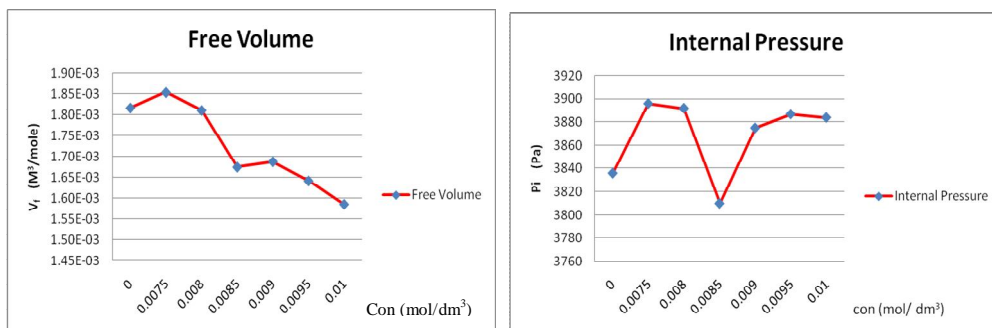


Fig. 3: Free Volume and Internal Pressure for aqueous L-Glutamic Acid at 303.15 K

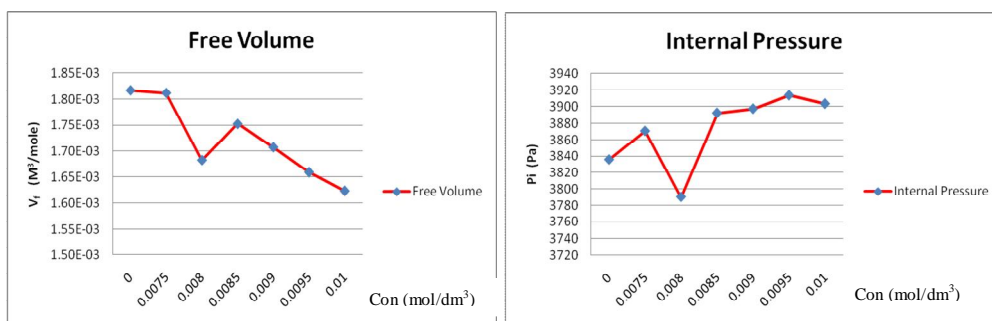


Fig. 4: Free Volume and Internal Pressure for aqueous L-Glutamine at 303.15 K

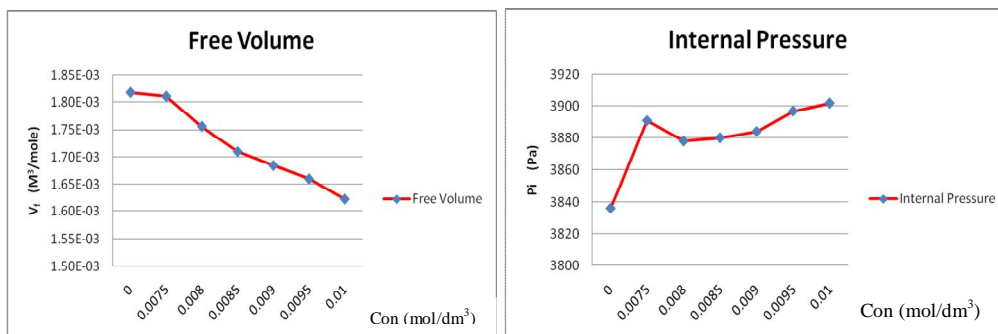


Fig. 5: Free Volume and Internal Pressure for aqueous L-Phenylalanine at 303.15 K

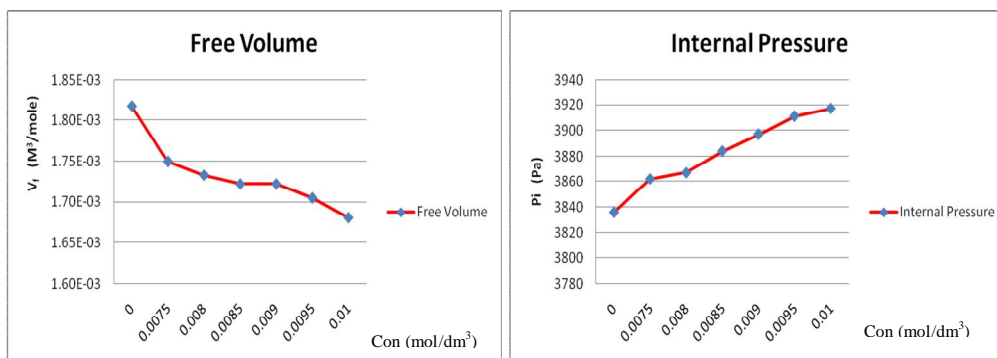


Fig. 6: Free Volume and Internal Pressure for aqueous L-Valine at 303.15 K

6. CONCLUSION

Different molecular interaction taking place in a solution is due to the combined effect of solvent structure, varying dielectric constant resulting from effect of the ions on structure of the solvents and steric hindrance of the solvent molecule.

7. REFERENCES

1. J.H. Hildebrand and R.L. Scott, Regular solution (Prentice-Hall, New Jersey, 1962)
2. J.H. Hildebrand and R.L. Scott, ed .3 Solubility of non-electrolytes (Reinhold, New York, 1964)
3. A.F.M. Barton, J. Chem. Educ. 48, 156 (1971)
4. C.V. Suryanarayana, Indian J. Pure Appl. Phys. 27, 751 (1989)
5. Digby D Macdonald and J.B. Hyne, Can. J. Chem. 49, 611 (1971)
6. M.R. J. Dack, Aust. J. Chem. 28, 1643 (1975)
7. M.R.J. Dack, J. Chem. Soc. Rev. (GB) 4, 211 (1975)
8. S.V. Subramanyam, T. Ramanujappa and E.S. Raja Gopal, Acustica 52, 125 (1983)
9. J.D. Pandey, n pant and B.R. Chaturvedi, Chem. Scr. 18, 224 (1981)
10. J.D. Pandey and R.L. Mishra, Acustica 39, 200 (1978)
11. J.D. Pandey and V. Tiwari, Z. Phys. Chem. (Leipzig) 262, 553 (1981)
12. L. Line Acevedo, Gracida C Pedrosa and Mignel Katz, J. Solution Chem. 19, 11 (1990)
13. E. Jr. Acree William, Thermodynamic properties of non-electrolyte solutions (Academic Press, Orlando, Florida, 1984) Ch. 8
14. J.D. Pandey, N. Pant, N. Agrawal and Shikha, Acustica 68, 225 (1989)
15. J.D. Pandey et al, Pramana- Journal of Physics, Vol 40, No. 2, 81-87 (Feb 1993)
16. Richard T.W. Chem. Rev. 2 (1925) 315.
17. Tammann G., Z. phys. Chem. 11 (1893) 676, 13 (1894) 174, 14 (1884) 613, 17 (1895) 620.
18. Heydewiller A. Phys. Z. 1 (1899) 114.
19. Dash U.N., Roy G.S. & Mohanty S., Indian J. Chem. 41A (2002) 2507.
20. Jacobson B. Acta Chem. Scand. 61 (1952) 1485.
21. Eyring H & Kinvaid J.F., Free volumes and free angles ratios of molecules in liquids, J. Chem. Phys. 6 (1938) 620.
22. Dash U.N., Roy G.S. & Mohanty S., Ultra Science, 15(2) (2003) 295.