MOLECULAR INTERACTION THROUGH FREE VOLUME AND INTERNAL PRESSURE OF AQUEOUS AMINO ACIDS AT 308.15 K

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Abstract:

The behavior of biologically active material at or near the physiological temperature (37˚ C or 98.6˚ F or 310.15 K) is of interesting and important for any living beings. By taking this consideration 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 308.15 K. (nearly equal to 310.15K) 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.

Introduction:

There is no absolute perfect body temperature. It varies from person to person as well as the place on or in the body where temperature is taken. Oral temperatures are slightly lower than rectal ones and skin temperatures are generally lower than oral ones. 98.6˚ F (37˚ C or 310.15 K) is a commonly accepted average. Hence average Physiological temperature i.e. normal human body temperature is often said to be 98.6 F degrees. The study of behavior of biologically active material at or near the physiological temperature (37˚ C or 98.6˚ F or 310.15 K) is of interesting and important towards the life cycle of mankind. Internal pressure is one of the most important parameter to discuss the molecular interaction. 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, fundamental properties of the liquid state has been studied initially by Hildebrand et al [1, 2] and subsequently by several workers [3-9]. 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 years [13] 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.

Material and Method

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

$Vf = (V/u3)(\gamma RT/M)3/2$--------------(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.

$Pint = bRT (k \eta / u)1/2\rho 2/3/M7/6$-------------(2)

Where b is packing factor, k is a constant independent of temperature having a value of 4.28 x 109 and η is the viscosity. The other symbols have their usual meaning. Thus (2) affords a method for estimating Pint form a knowledge of η, ρ and u. 3. Experimental 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 of were made with doubled distilled water. Densities, Viscosities and ultrasonic velocities were measured at 308.15 K. Densities were determine with Density Bottle with plunger method. Viscosities were determined with Oswald Viscometer and Ultrasonic Velocities with Pluse Echo Overlap Method using Innovative Instrument-102 (AUAR) along with Ultrasonometer (4 MHz) and Universal Time & Frequency Counter.

Result and Discussion:

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 determined as shown in Table1, Table 2 , Table 3, Table 4 ,Table 5 and Table 6 Free volume and internal pressure values for all pure liquid system were calculated from equ. (1) and (2) and are given in column 6 and 7 respectively of all Tables. Fig (1),(2), (3) ,(4) (5) and (6)showing respectively the variation of Free Volume (Vf) and Internal Pressure(Pint) with different concentration of L-Alanine, L-Aspartic Acid, L-Glutamic Acid, L-Glutamine, L-Phenylalanine and L-Valine at 308.15K 5. Discussion Propagation of ultrasound in a medium is concentration dependent. Hence , ultrasonic velocity and attenuation were measured for various concentration of pure amino acids various ultrasonic parameters calculated based on the ultrasonic velocity and density of these solution are given in tables 1 to 6 and corresponding profile are shown in figures 1 to 6. There may be many acoustical parameters which can be used for understanding the molecular interaction but here we most concentrated on free volume and internal pressure 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

(Pi) increases with concentration. The free volume (Vf) is found to decrease with concentration. Both Pi and Vf 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 Vf (increase of Pi) indicates the formation of hard or tight solvation layer around the ion and increase of Vf (decrease of Pi) 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.

Observations and Graphs :

Table: 1. ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Alanine (Mol.Wt. 89.09) at 308.15K

S.No.	**Molarities**	**Ultrasonic Velocity (u) (m/s)**	**Density (ρ) (Kg/m3)**	**Viscosity (η)(Pa s)**	**Free Volume (Vf) (m3/mole)**	**Internal Pressure (*P*int) (Pa)**
1	0.0000	1522.73	0.99393	0.7200	1.811E-03	3.805E+03
2	0.0075	1518.51	1.00372	0.72974	1.781E-03	3.825E+03
3	0.0080	1519.77	1.00173	0.73495	1.786E-03	3.840E+03
4	0.0085	1522.44	1.00834	0.74213	1.749E-03	3.847E+03
5	0.0090	1537.45	1.02697	0.73754	1.590E-03	3.793E+03
6	0.0095	1530.39	1.01320	0.75106	1.664E-03	3.854E+03
7	0.0100	1532.88	1.01590	0.75606	1.646E-03	3.860E+03

Table: 2. ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L- Aspartic Acid (Mol.Wt. 133.10) at 308.15K

S.No.	**Molarities**	**Ultrasonic Velocity (u) (m/s)**	**Density (ρ) (Kg/m3)**	**Viscosity (η)(Pa s)**	**Free Volume (Vf) (m3/mole)**	**Internal Pressure (*P*int) (Pa)**
1	0.0000	1522.73	0.99393	0.72	1.812E-03	3.805E+03
2	0.0075	1506.77	1.00283	0.73385	1.821E-03	3.853E+03
3	0.0080	1521.13	1.00140	0.73344	1.784E-03	3.836E+03
4	0.0085	1543.16	1.01474	0.70874	1.666E-03	3.728E+03
5	0.0090	1540.45	1.01231	0.76012	1.641E-03	3.867E+03
6	0.0095	1544.35	1.01978	0.76809	1.601E-03	3.873E+03
7	0.0100	1555.55	1.02086	0.77698	1.568E-03	3.880E+03

Table: 3. ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L- Glutamic Acid (Mol.Wt. 147.13) at 308.15K

S.No.	**Molarities**	**Ultrasonic Velocity (u) (m/s)**	**Density (ρ) (Kg/m3)**	**Viscosity (η)(Pa s)**	**Free Volume (Vf) (m3/mole)**	**Internal Pressure (*P*int) (Pa)**
1	0.0000	1522.73	0.99393	0.72	1.812E-03	3.805E+03
2	0.0075	1509.83	1.00498	0.72832	1.802E-03	3.832E+03
3	0.0080	1519.57	1.00622	0.73686	1.768E-03	3.841E+03
4	0.0085	1547.00	1.02667	0.72249	1.608E-03	3.745E+03
5	0.0090	1532.50	1.01211	0.74843	1.706E-03	3.848E+03
6	0.0095	1534.23	1.01511	0.75944	1.689E-03	3.870E+03
7	0.0100	1541.75	1.01621	0.76465	1.664E-03	3.873E+03

Table: 4. ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Glutamine (Mol.Wt. 146.15) at 308.15K

S.No.	**Molarities**	**Ultrasonic Velocity (u) (m/s)**	**Density (ρ) (Kg/m3)**	**Viscosity (η)(Pa s)**	**Free Volume (Vf) (m3/mole)**	**Internal Pressure (*P*int) (Pa)**
1	0.0000	1522.73	0.99393	0.72	1.811E-03	3.805E+03
2	0.0075	1521.15	0.99888	0.72432	1.795E-03	3.815E+03
3	0.0080	1532.70	1.01299	0.71287	1.701E-03	3.753E+03
4	0.0085	1525.11	1.00950	0.74927	1.738E-03	3.862E+03
5	0.0090	1527.32	1.01870	0.75846	1.693E-03	3.871E+03
6	0.0095	1530.25	1.02537	0.77360	1.657E-03	3.898E+03
7	0.0100	1529.97	1.02659	0.78102	1.653E-03	3.915E+03

Table: 5. ultrasonic velocity, density, viscosity, free Volume and Internal Pressure for aqueous L-Phenylalanine (Mol.Wt. 165.19) at 308.15K

S.No.	**Molarities**	**Ultrasonic Velocity (u) (m/s)**	**Density (ρ) (Kg/m$_3$)**	**Viscosity (η)(Pa s)**	**Free Volume (V$_f$) (m$_3$/mole)**	**Internal Pressure (*P*$_{int}$) (Pa)**
1	0.0000	1522.73	0.99393	0.72	1.811E-03	3.805E+03
2	0.0075	1511.29	1.03954	0.76926	1.652E-03	3.892E+03
3	0.0080	1517.21	1.04834	0.77301	1.602E-03	3.892E+03
4	0.0085	1520.01	1.04047	0.76952	1.625E-03	3.881E+03
5	0.0090	1522.83	1.04751	0.77616	1.590E-03	3.886E+03
6	0.0095	1528.75	1.05506	0.77863	1.547E-03	3.876E+03
7	0.0100	1533.51	1.05796	0.77799	1.525E-03	3.865E+03

Table: 6. ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Valine (Mol.Wt. 117.15) at 308.15K

S.No.	**Molarities**	**Ultrasonic Velocity (u) (m/s)**	**Density (ρ) (Kg/m3)**	**Viscosity (η)(Pa s)**	**Free Volume (V_f) (m3/mole)**	**Internal Pressure (P_{int}) (Pa)**
1	0.0000	152273	0.99393	0.72	1.811E-03	3.805E+03
2	0.0075	150752	1.00588	0.73545	1.804E-03	3.852E+03
3	0.0080	151842	1.00409	0.74039	1.780E-03	3.853E+03
4	0.0085	152633	1.00920	0.75139	1.735E-03	3.865E+03
5	0.0090	153185	1.01212	0.75453	1.707E-03	3.863E+03
6	0.0095	153367	1.01642	0.76084	1.684E-03	3.871E+03
7	0.0100	153771	1.01758	0.76740	1.668E-03	3.882E+03

L-Alanine

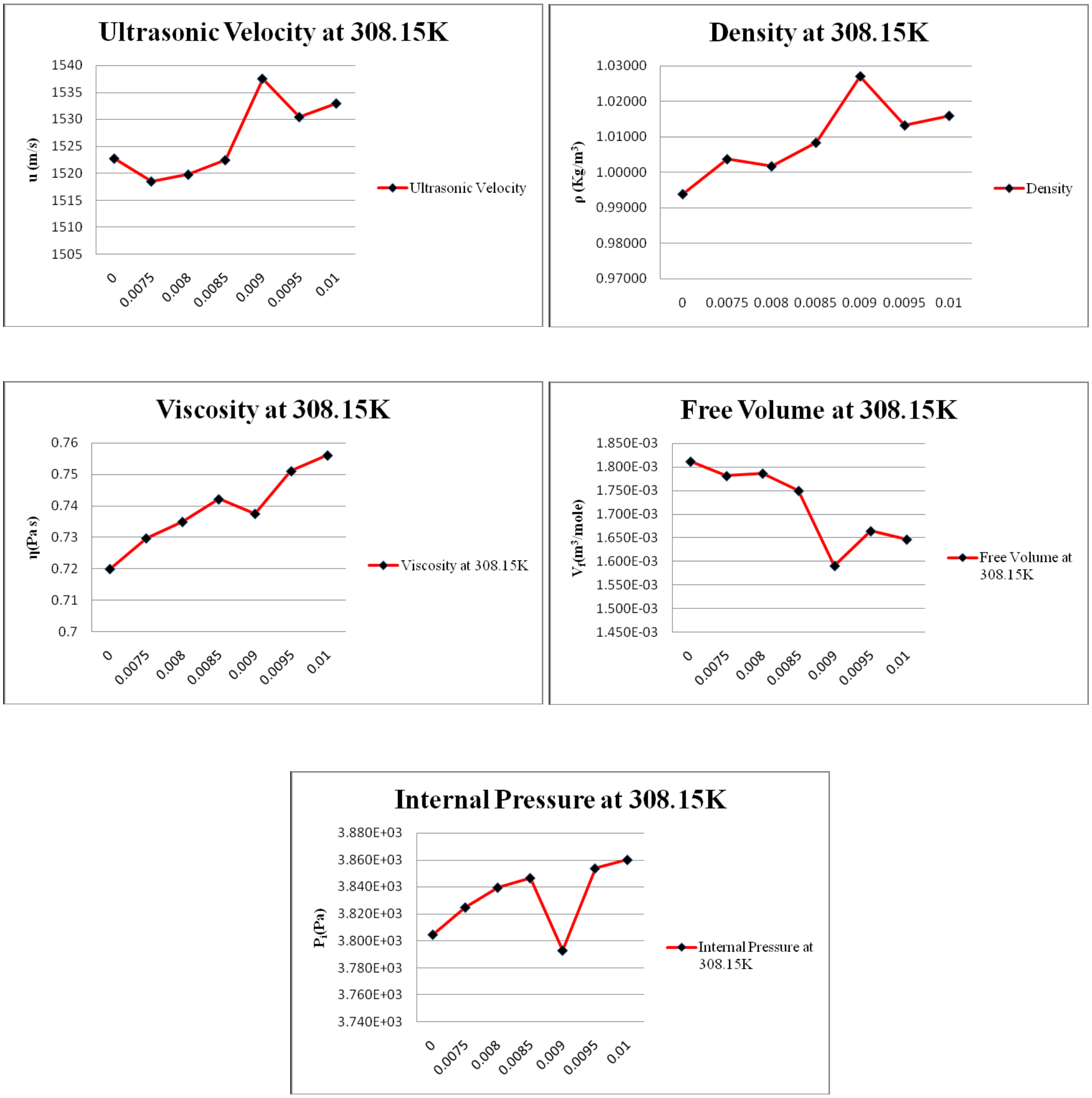
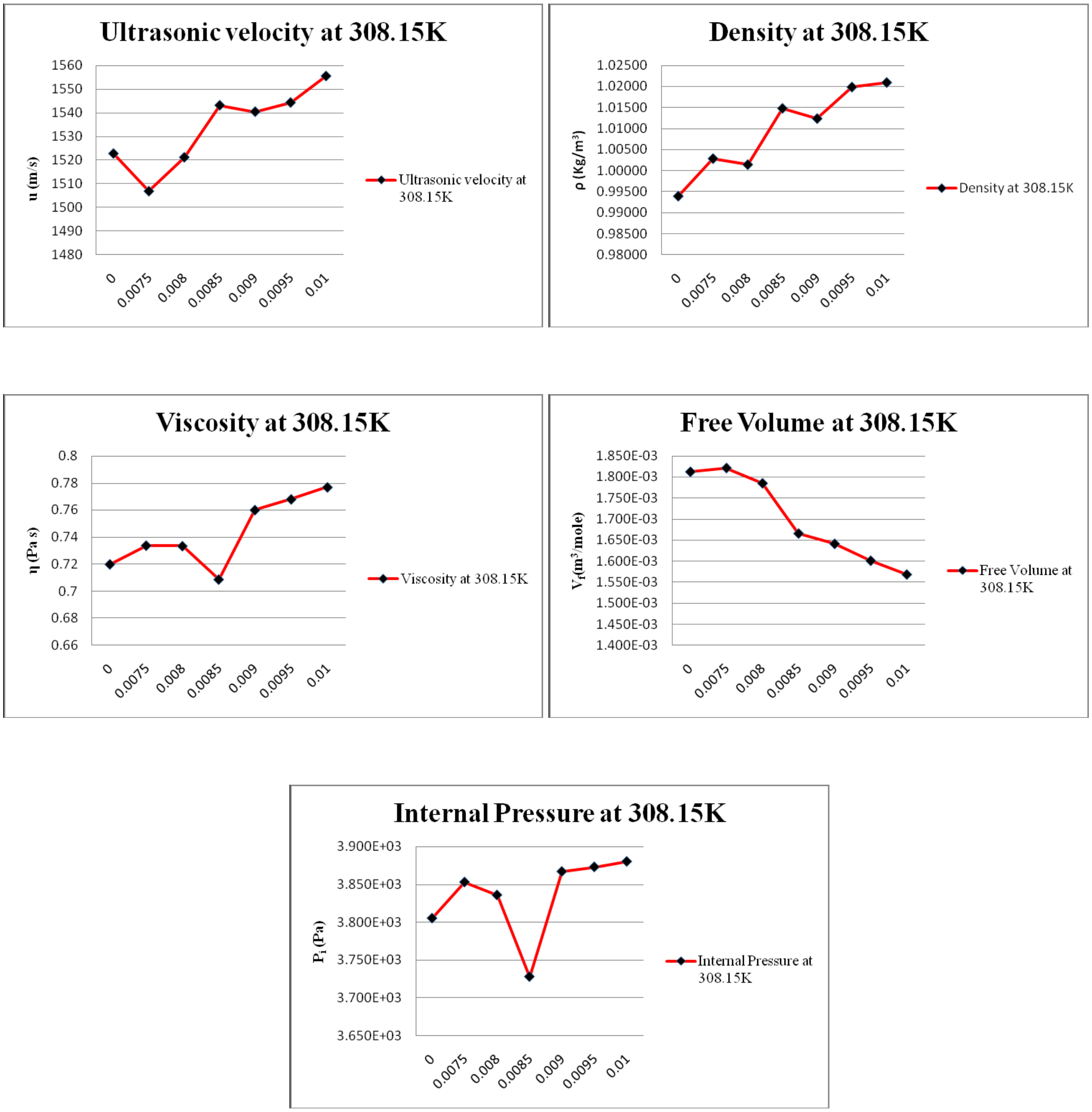


Fig 1: ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Alanine at 308.15K

L-Aspartic Acid


Ultrasonic velocity at 308.15K

Density at 308.15K

Viscosity at 308.15K

Free Volume at 308.15K

Internal Pressure at 308.15K

Fig 2: ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Aspartic Acid at 308.15K

L-Glutamic Acid

Fig 3: ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Glutamic Acid at 308.15K

L-Glutamine

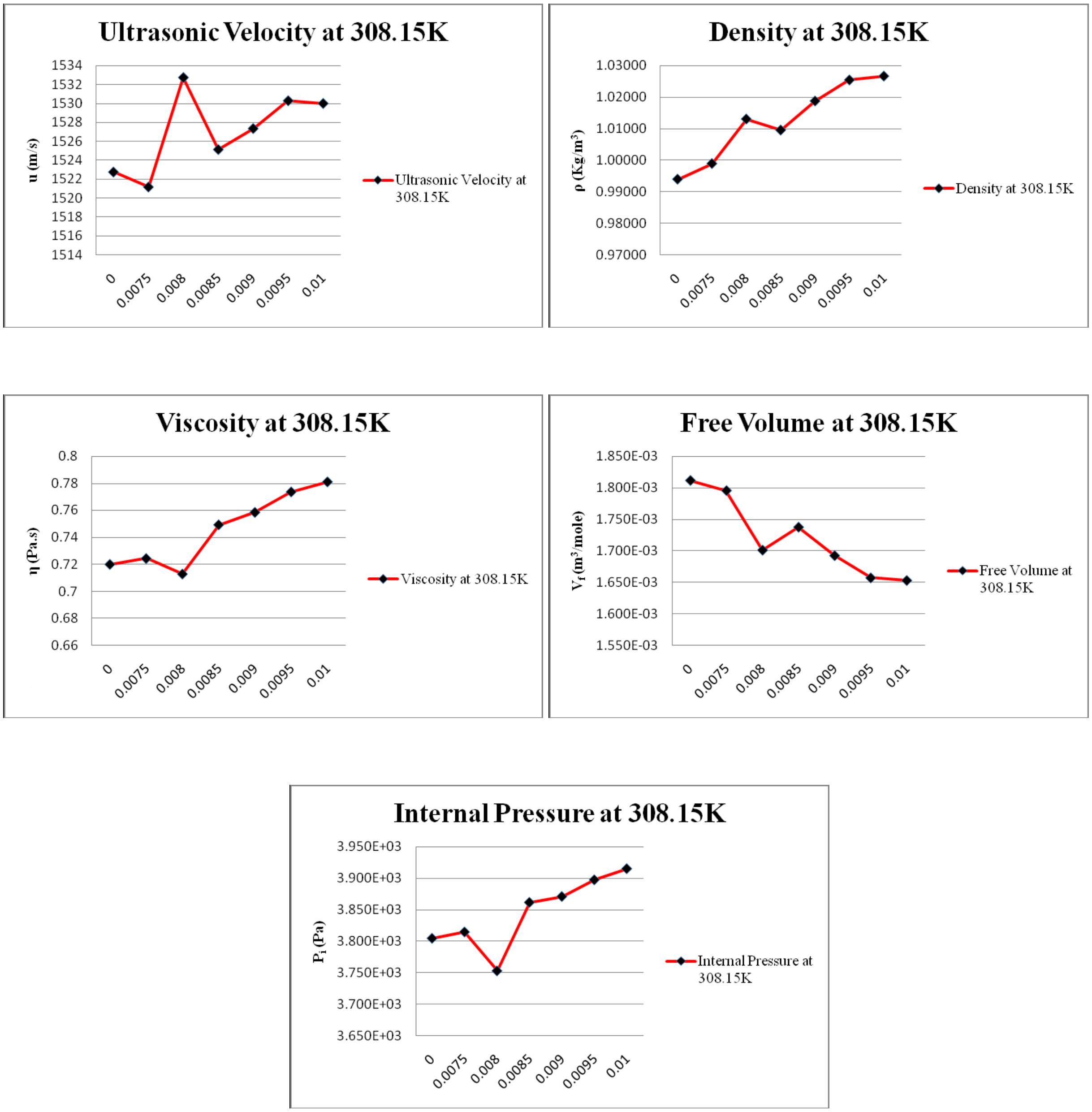


Fig 4: ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Glutamine at 308.15K

L-Phenyllanine

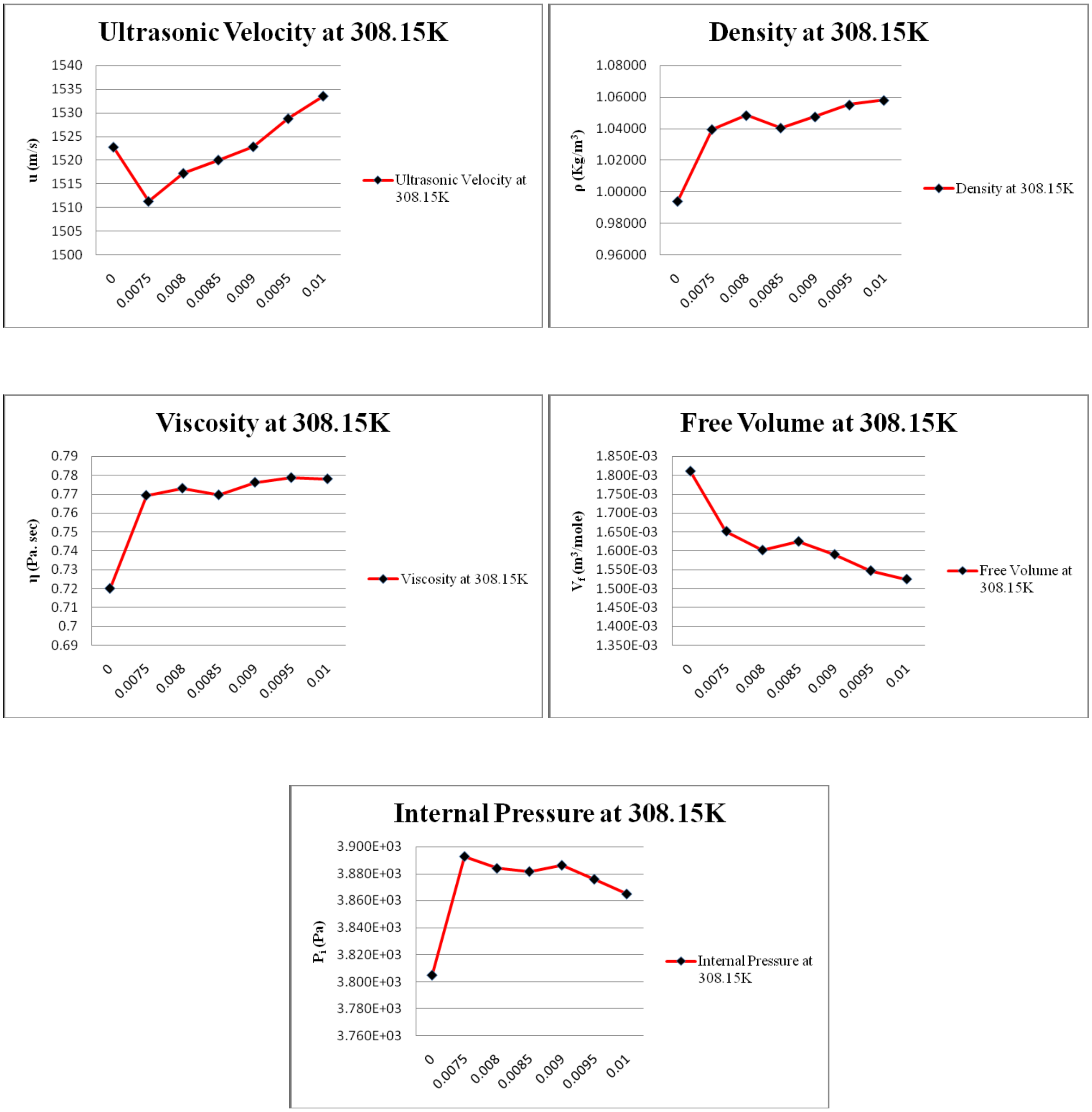


Fig 5: ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Phenyllanine at 308.15K

L-Valine

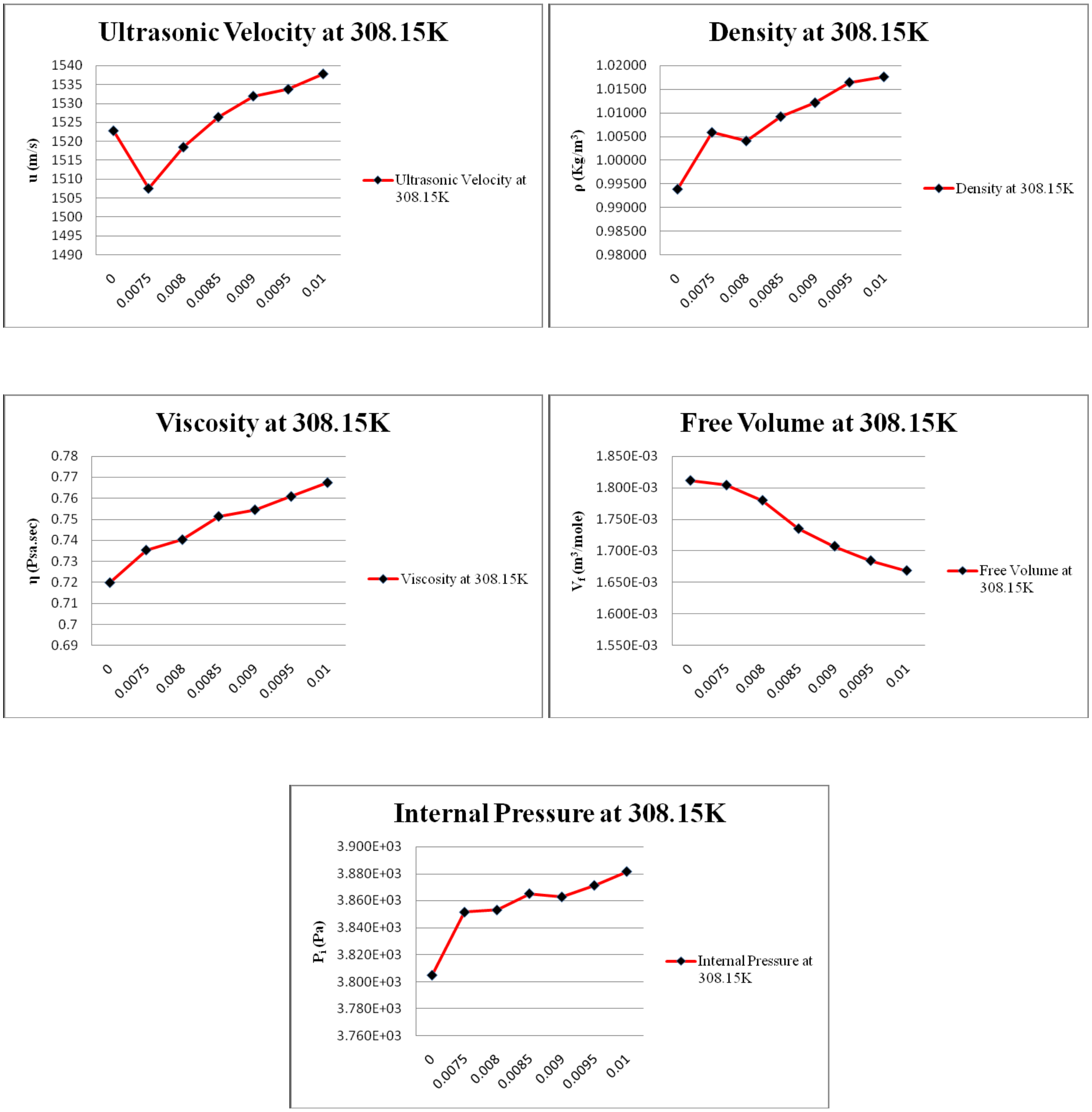


Fig 6: ultrasonic velocity, density, viscosity, free volume and Internal Pressure for aqueous L-Valine at 308.15K

Conclusion

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. We conclude that our method has three important areas of application: 1) They provide a means to measure acoustical and viscoelastic properties of biologically active material. 2) They provide a simple basis for investigating the molecular interaction between bio materials 3) They provide reliable measures of absorption and velocity dispersion that can be used to investigate the testability of adhered structures by ultrasonic means.

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