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Molecular Interactions by Ultrasonic Measurements in Aqueous and 10% Ethanol-Water Solutions of MYO-INOSITOL At 298.15K

S. A. Shah
Department of Chemistry, Anand Niketan College, Anandwan, Warora, Maharashtra, India

ABSTRACT

Density(ρ), ultrasonic velocity(U) and viscosity(η) have been measured experimentally for aqueous solution of myo-inositol at concentration range (0.1 M- 0.9 M) and 10% ethanol-water solutions of meyo-inositol at concentration range(0.05M-0.45M) at temperature (298.15K).The acoustic parameters such as adiabatic compressibility(β),free length(L_f), free volume(V_f), relaxation time(τ) and internal pressure have been worked out. The results are correlated in terms of non-covalent molecular interaction between the constituents of solutions.

Keywords : Ultrasonic velocity, Acoustic parameters, Meyo-Inositol

I. INTRODUCTION

Ultrasonic velocity of pure liquids and liquid mixtures are basically related to the non-covalent molecular interactions (hydrogen bonding, Vander Waal's forces and dispersion forces) between molecules and atoms. The speed and efficiency of the transmission is sensitive to the nature of the bonds and the masses of the molecules present in the liquid mixtures and hence composition of system [1]. The ultrasonic technique can be used as method for providing information about physicochemical properties of the materials. The principle used in this technique is that the ultrasonic wave can be changed by the intermolecular interactions (ion-dipole, dipole-dipole, dipole-induced dipole, and hydrogen bonding and dispersion forces) of the sample while it travels through the sample. By compare the incident and resultant ultrasonic wave the structure in the sample can be concluded [2].

Chemistry and biology of meyo-inositol derivatives has been investigated widely in the recent past due to the association of phosphoinositols in cellular signal transduction mechanisms [3] and anchoring of certain proteins to cell membranes [4]. Although a bewildering array of myo-inositol phosphates and their lipid derivatives have been identified and / or isolated from plant as well as animal sources, the biological roles played by many of them is not yet clearly understood. However, receptors and effectors involved in various stages of phosphoinositol based signal transduction pathways remain potential targets for pharmacological intervention in states of disease[5].These developments in biology and medicine have necessitated the efficient synthesis of naturally occurring phosphoinositols and their synthetic analogs. Myo-Inositol is a cyclic sugar alcohol. It is also known as cyclitol. The chemistry of the cell is controlled by myo-inositol. There should be

communication between outer and inner environment of a cell. The calcium channels of cell membrane can be opened by the derivative of myo-inositol (inositol-1,4,5 triophosphate). It allows the calcium ions to enter into the extracellular fluids[6].The chemistry and biology of myo-inositol derivatives has been investigated widely in the recent past due to the association of phosphoinositols in cellular signal transduction mechanisms [7] and anchoring of certain proteins to cell membranes [8].
The ultrasonic study of this molecule in aqueous and aqueous alcoholic medium is very important for understanding the behaviour water structures, biomolecular recognition and medicinal use.

II. METHODS AND MATERIAL

The solutions of myo- Inositol was prepared by dilution method. All the chemicals are of AR grades of 99.99 % purity. Composition range of myo-inositol is from 0.1 M to 0.9M in water and for myo-inositol the concentration range from 0.05M-0.45M (solubility of myo-inositol lower in 10% ethanol-water solvent system).
The ultrasonic velocity in the liquid mixtures have been measured by means of ultrasonic interferometer (Mittal type: Model: M-83) functioning at frequency 2MHz with an overall accuracy of ±0.1 m/s, an electronically digital operate constant temperature water bath has been used to flow water through the double walled measuring cell, made up of a steel containing the experimental solution at the preferred temperature. For weighing, an electronic digital balance having an accuracy of ±0.1 mg was used. An Ostwald's viscometer was used for the measurement of viscosity of liquid mixtures with an accuracy of 0.0001Nsm2. The viscometer was calibrated before used. Time flow of water and liquid solutions were measured. Densities were determined using specific gravity bottle by relative measurement method with accuracy of ±0.1 kg.m^{-3}.

III. RESULTS AND DISCUSSION

The experimental parameters and derived parameters presented in figure myo-inositol respectively. From these parameters, the acoustic parameters such as adiabatic compressibility(β),free length(L_f), free volume(V_f), relaxation time(τ) and internal pressure have been worked out and correlation of intermolecular interactions were established by plotting graphs.
By using density, ultrasonic velocity and viscosity of aqueous and 10% ethanol-water solution of myo-inositol, various acoustic parameters such as(β_a), intermolecular free length (L_f) , free volume (V_f),internal pressure (π_i), relaxation time (τ), were calculated. The experimental parameters as well as derived acoustic parameters have been discussed in the light of molecular association.

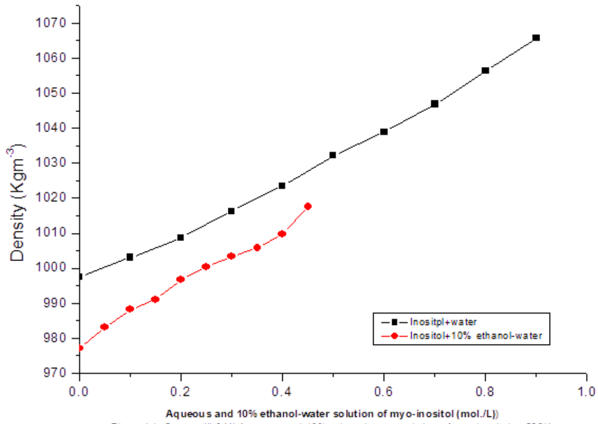

Figure (a): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K.

From fig.1.1 (a) the experimental values of density of aqueous and 10% ethanol-water solution of myo-insitol is found to increase with increase in concentration of solutes (myo-inositol), suggesting that the strength of interaction is enhanced. The increasing trend of density with increasing solute concentration indicates more number of components of the medium. Thus, it leads to closed packing of the medium and enhanced the intermolecular interactions. On comparing these values for aqueous and in 10% ethanol-water water solvent systems it is found that density is minimum in 10% ethanol-water. It may be due to number of molecules per unit area is lesser as compare to aqueous medium and packing of solute molecules greater in aqueous medium than 10% ethanol-water solvent system.

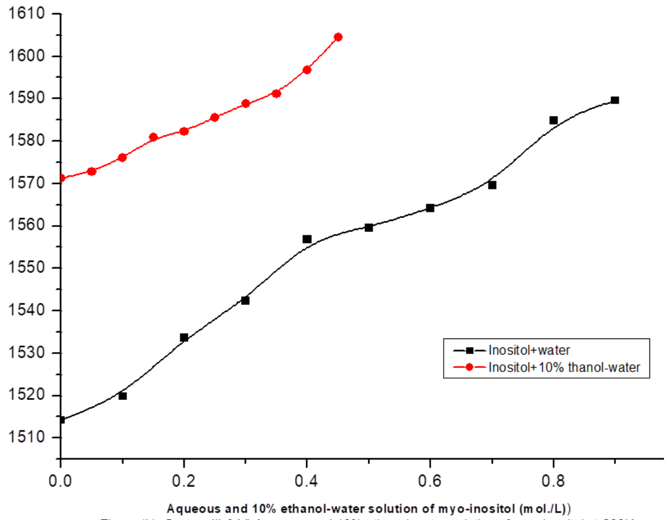

Figure (b): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K.

From fig.1.1 (b) the experimental values of ultrasonic velocity of aqueous and 10% ethanol-water solution of myo-inositol is found to increase with increase in concentration of solutes (myo-inositol), suggesting that the strength of interaction is enhanced. The increasing trend of ultrasonic velocity with increasing solute concentration indicates more number of components of the medium. Thus, it leads to closed packing of the medium and enhanced the intermolecular interactions [9-10]. On comparing these values for aqueous and in 10% ethanol-water water solvent systems it is found that ultrasonic velocity is maximum in 10% ethanol-water. It may be due to strong hydrogen bonding between solute and solvent molecules as compare to aqueous medium and strength of interaction is greater in 10% ethanol-water solvent system than aqueous medium. It may be due to like nature of myo-inositol and alcohol molecules and strong interaction between ethanol and water molecules as compare to the interaction among the indusial molecules.

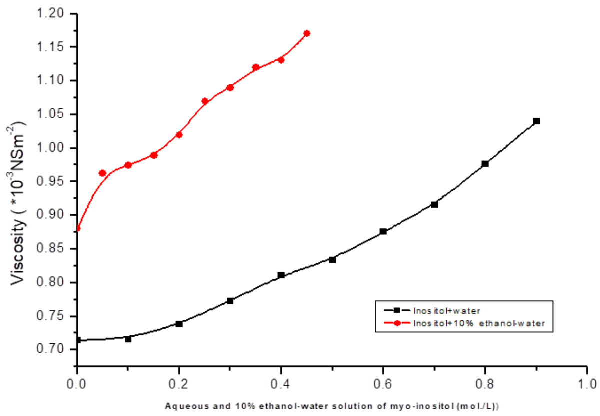

Figure (c): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K.

From fig.1.1 (c) the coefficient of viscosity is a fundamental property of liquids that decides the inner nature of the liquids. The coefficient of viscosity provides much more information about the medium. The variations of coefficient of viscosity depend on the surface area of the molecules, relative degrees of freedom (rotational, vibrational and translational) of the molecules and the molecular geometry [11-12]. The experimental values of viscosity of aqueous and 10% ethanol-water solution of myo-insitol is found to increase with increase in concentration of solutes (myo-inositol), suggesting that the strength of interaction is enhanced. The increasing trend of viscosity with increasing solute concentration indicates more number of components of the medium. Thus, it leads to closed packing of the medium and enhanced the intermolecular interactions. On comparing these values for aqueous and in 10% ethanol-water water solvent systems it is found that coefficient of viscosity is maximum in 10% ethanol-water. It may be due to strong hydrogen bonding between solute and solvent molecules as compare to aqueous medium and strength of interaction is greater in 10% ethanol-water solvent system than aqueous medium. It may be due to like nature of myo-inositol and alcohol molecules (like nature molecules have greater affinity) and strong interaction between ethanol and water molecules (ethanol-water) as compare to the interaction among the indusial (water-water and ethanol-ethanol) molecules.

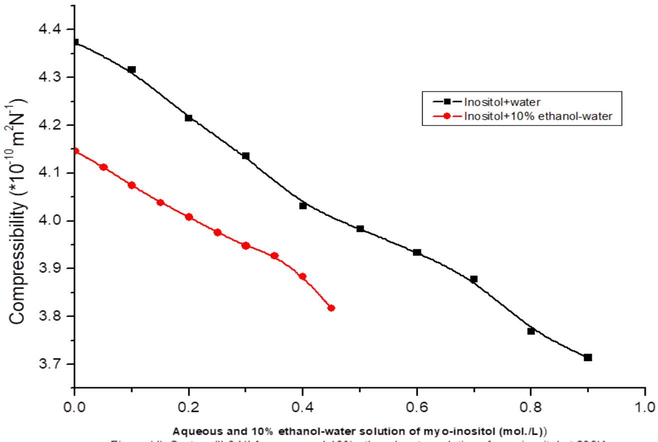

Figure (d): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K.

From figs.1.1 (d) and (e), the decrease in compressibility and free length implies that there is enhanced molecular association in this system upon addition of solute and less available free space between the components of the solution. The new complexes formed due to molecular association become more compact and less compressible. These also suggest that the compressibility and free length of the solution is less than that of solvent. The magnitude of compressibility depends on the electrostriction. It throws light on the hydrophobic-hydrophilic interactions in the medium. Negative values indicate hydrophobic interaction and loss of structural compressibility due to increased population of hydrogen bonded solvent molecules. This decrease trend in compressibility and free length with increase in concentration of solute (myo-inositol) indicate enhancement of solute-solvent interaction through intermolecular hydrogen bonding and dispersion forces[13-15]. If the compressibility and free length values are higher, it suggests that the medium is loosely packed and lower values indicate maximum interactions.

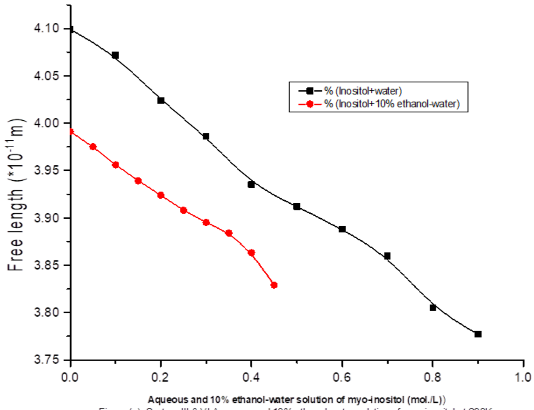

Figure (e): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K.

From fig.1.1 (d) and (e), it is found that the trend revealed by adiabatic compressibility and free length is decreased with increase in concentration for studied molecule (myo-inositol) in 10% ethanol-water system compare to the aqueous medium. It may be due to like nature of myo-inositol and alcohol molecules (like nature molecules have greater affinity) and strong interaction between ethanol and water molecules (ethanol-water) as compare to the interaction among the indusial (water-water and ethanol-ethanol) molecules.

Free volume and internal pressure:

Free volume is the average volume in which the central molecule can move inside the hypothetical cell due to repulsive interaction of neighbouring molecules. Monomer size space present in the system due to irregular packing of solvent molecules also called as free volume.

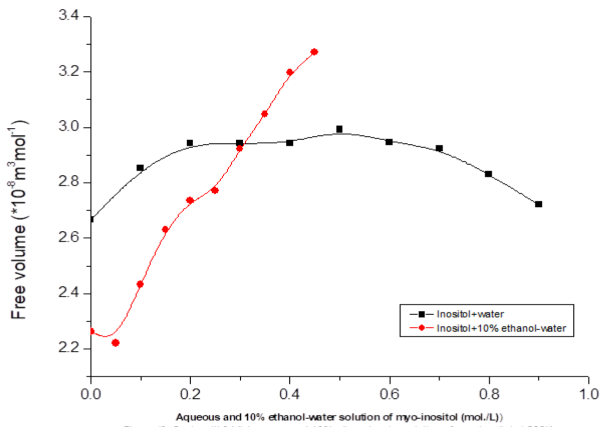

Figure (f): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K.

From fig. 1.1 (f) values of free volume for 10% ethanol-water solutionof myo-inositol is found to increase with increase in concentration suggest that there is weak interaction between solute and solvent molecules. The free volume of the solution depends on the coefficient of viscosity as compare to density and ultrasonic velocity of the medium. The increase in free volume may be due to loosening of cohesive forces which result into breaking up structure of solvent system [16]. The decrease of free volume with concentration may be due to strong association between solute and solvent molecules through intermolecular hydrogen bonding and dispersion forces.

The free volume of aqueous Myo-inositol solution increases with increase in Myo-inositol concentration up to 0.6M and then decrease up to end suggest that from 0.1 to 0.6 molar concentration solution there is weak interaction between solute and solvent molecules. The enhancement of solute –solvent interaction takes place from 0.7 to 0.9 molar concentrations. The increase in free volume may be due to loosening of cohesive forces which result into breaking up structure of water. The decrease of free volume at higher concentration range may be due to strong association between solute and solvent molecules through intermolecular hydrogen bonding. Free volume and internal pressure inversely correlated with other [17].

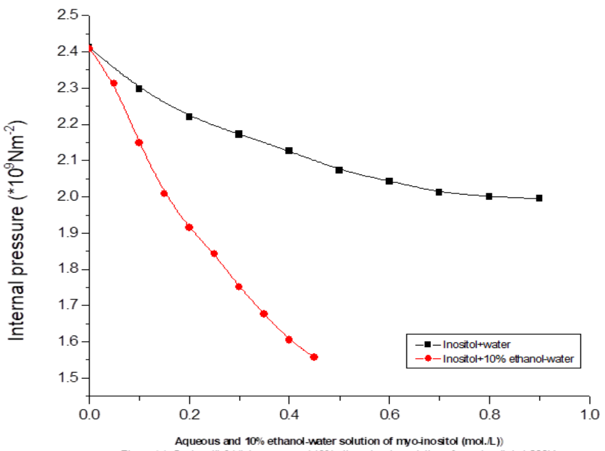

Figure (g): System III & VI Aqueous and 10% ethanol-water solution of myo-inositol at 298K

From fig. 1.1 (g) the internal pressure of Myo-inositol solution is found to be decreases with increase in Myo-inositol concentration in both solvent systems, which indicates decrease in cohesive forces. In aqueous medium the internal pressure is found to be maximum as compare to 10% ethanol-water system, suggesting strong solute-solvent interaction in aqueous medium due strong intermolecular hydrogen bonding. In 10% ethanol-water solvent system cohesive force is found to decrease, this may be due to Repulsive forces among the solute and solvent molecules due to presence of ethyl group of ethanol molecules. Although the values of ultrasonic velocity, density, viscosity, adiabatic compressibility and free length attribute the predominance of solute-solvent interaction, the decrease in internal pressure with concentration indicates the presence of solute-solute interaction.

The relaxation time measure the closed packing of the medium. If the medium is loosely packed, it is easy to disrupt the medium and changing the equilibrium of the system. If the medium is closed packed, it is difficult to disrupt the medium and changing the equilibrium [18-19]. From fig. 1.1 (h) the increase of relaxation time with the Myo-inositol concentration strongly supports the intermolecular association through dipole-dipole (hydrogen bonding) interaction between solute and solvent molecules. When Myo-inositol is added in aqueous and 10% ethanol-water, Myo-inositol molecules may break the structure of associated solvent molecules and forms the solute-solvent complex. The Myo-inositol-water and Myo-inositol-ethanol hydrogen bonding is more favourable than water-water and water-ethanol hydrogen bonding. The Myo-inositol-water and ethanol bonding is enhanced due to extra bonding (dipole-dipole, dipole induced-dipole). Due to formation of complexes in the solution, particle size and masses increased. This leads to increase the cohesive forces, frictional forces and reduced the relative motion and rotation of freedom of the molecules of the Myo-inositol solution. When the Myo-inositol concentration increase in both solvent system, the number of hydroxyl (-OH) groups available for hydrogen bond formation also increase and result into large number of hydrogen bonds between solute and solvent molecules. Relaxation time is found to be greater for 10% ethanol-water solvent system compare to the aqueous medium. This may be the effect of solvent system. The relaxation time is minimum for pure aqueous medium as compare to the 10% ethanol-water system.

IV.CONCLUSION

Molecular interaction depends on solvent systems. In the above present work, myo-inositol molecule strong molecular interaction in 10% ethanol-water system compare to aqueous myo-inositol. It is also concluded that ethanol-water molecules have greater molecular interaction than water-water molecules. In 10% ethanol-water system, solvent-solvent molecules have greater interaction than solute-solvent interactions.

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