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Ultrasonic and Thermodynamic Investigation of Molecular Interactions in Acetylcholine with 1-Butanol Binary Mixtures at 303 K

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ABSTRACT: Understanding how molecular interactions affect molecular association in solution can be done by examining the physicochemical properties of binary liquid mixtures. This paper presents the ultrasonic velocity (U), density and viscosity (η) of the binary mixture of acetylcholine with 1-butanol measured by experiment at a temperature of 303 K and over the full range of mole fractions. Using the measurements, we calculated the following acoustical and thermodynamic parameters for each mixture of 1-butanol with acetylcholine: adiabatic compressibility (β), intermolecular free length (L_f), acoustic impedance (Z) and free volume (V_f). A decrease in ultrasonic velocity with increasing mole fraction of 1-butanol combined with a corresponding increase in viscosity and density shows the presence of strong molecular interactions between the two components. Evaluation of the derived parameters suggests hydrogen bonding and dipole-dipole interactions between acetylcholine and 1-butanol molecules. Method of ultrasonic investigation gives the structure and behavior of biological molecules in an alcoholic medium to achieve greater insight into molecular association in biologically significant solvent systems.

KEYWORDS: Ultrasonic velocity, Molecular interactions, Binary liquid mixtures, Acetylcholine, 1-Butanol.

I. INTRODUCTION

Analyzing how molecules interact in two-component solutions forms the basis for comparing thermodynamic, structural, and transport characteristics of liquids. Because the way sound travels through a liquid depends on the intermolecular forces present in the liquid (i.e., how tightly or loosely packed the molecules are), ultrasonic techniques offer a sensitive and reliable means for investigating intermolecular interactions. The measurement of the speed of sound, density, and viscosity of a liquid will allow for the determination of derived thermodynamic parameters, such as the adiabatic compressibility, the intermolecular free length, and the acoustic impedance of the liquid. These parameters provide information about the extent of molecular association, the amount of hydrogen bonding, and the ability of the molecules to move around and re-arrange themselves when mixed with other molecules [1-3].

Acetylcholine plays an important role in numerous physiological processes, including the transmission of neural signals. Since acetylcholine is one of the most important neurotransmitter compounds and Acetylcholine is also a common research subject in both pharmacology and biochemistry. Therefore, it would be of great interest to understand how acetylcholine interacts with other molecules in different solvents, as this could impact its function as a neurotransmitter. Alcohols are used extensively in both the pharmaceutical and chemical industries because of their ability to form hydrogen bonds and their amphiphilic properties. When you consider the length of the hydrophobic alkane chain in primary alcohols, you can see that 1-butanol has a longer chain than the shorter-chain alcohols [4-7]. This has an important effect upon molecular packing, the polarity of the solvent, and the intermolecular forces acting on the alcohols in a given solution. Nevertheless, there have been few extensive studies looking into the affects that both Acetylcholine and higher alcohols (1-Butanol) have on each other. The investigations will allow for more clear understanding of complete interaction mechanisms based on both chain length and polarity of the molecules being studied [8-10].

As a result, this study will look at molecular interactions between Acetylcholine and 1-Butanol using ultrasonic testing methods. To determine the acoustic and thermodynamic parameters associated with the intermolecular forces present in this system, ultrasonic velocity, density, and viscosity will be measured at 303 K. Ultrasonic studies of alcohol mixtures

have provided valuable insight into the amount of hydrogen bonding, how dipoles interact, and how the underlying structure affects the interactions between the molecules in binary mixtures.

II. MATERIALS AND METHODS

An ultrasonic interferometer supplied by Mittal Enterprises, New Delhi, to measure the speed of sound (or ultrasonic velocity) to an accuracy of $\pm 2 \text{ ms}^{-1}$ at a frequency of 2 MHz. The temperature of the liquid mixtures was maintained at $303 \pm 0.1 \text{ K}$ using a thermostatically controlled water bath. All chemicals used will be of analytical reagent grade, sourced from SD fine chemicals, India, and used without further purification. All liquid mixtures in this study were made according to the mole fraction method, with a range of 0.1 to 0.7 corresponding to the different concentrations of the binary liquid mixtures created from the respective components of each experiment. Acetylcholine in chlorine is purchased from sigma chemical Ltd. It is dissolved in acetone and made stock solution. The density of pure liquids and liquid mixtures are determined using a Specific Gravity bottle by relative measurement method with an accuracy of $\pm 0.1 \text{ mg}$. An Ostwald's Viscometer which is 10ml capacity is used for the viscosity measurement of pure liquids and liquid mixtures.

From the measured parameters, the following acoustical quantities were calculated:

Ultrasonic velocity $U = n\lambda$ in ms^{-1}

Adiabatic Compressibility $\beta = \frac{1}{\rho U^2}$ in $\text{ms}^2 \text{kg}^{-1}$

Intermolecular Free Length $L_f = K_T \sqrt{\beta}$ $\text{kg m}^{-2} \text{s}^{-1}$

Where K_T is the temperature dependent Jacobson constant, $K_T = 2.075 \times 10^{-6} \text{ m}$ at 303K

Acoustic Impedance $Z = \rho U$ $\text{kgm}^{-2}\text{s}^{-1}$

Free Volume $V_f = \left(\frac{MU}{K\eta}\right)^{\frac{3}{2}}$ $\text{m}^3 \text{mol}^{-1}$

Where ρ = density, U = ultrasonic velocity, η = viscosity and M = effective molecular weight

III. RESULTS AND DISCUSSION

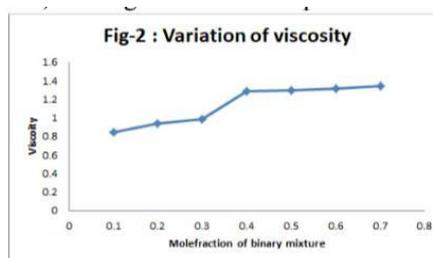
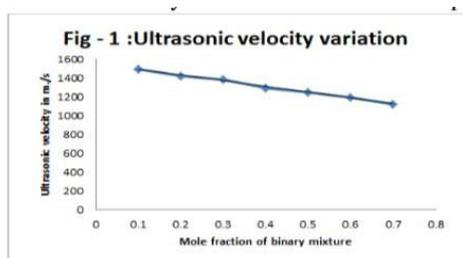
The experimentally measured values of ultrasonic velocity (U), density (ρ), and viscosity (η) for the binary mixture of acetylcholine with 1-butanol at 303 K are presented in Table 1. From these experimental data, several acoustical and thermodynamic parameters such as adiabatic compressibility (β), intermolecular free length (L_f), acoustical impedance (Z), free volume (V_f), and relaxation time (τ) were calculated to understand the nature of molecular interactions in the system.

Table 1 Value of ultrasonic velocity (U), Density (ρ) and Viscosity (η).

Mole fraction		For 1-Butanol with Acetylcholine						
X1	X2	U (m/s)	$\eta \times 10^3$ Ns m^{-2}	ρ Kg m^{-3}	$\beta \times 10^{-10}$ $\text{ms}^2 \text{N}^{-1}$	$L_f \times 10^{-10}$ m	$V_f \times 10^{-8}$ $\text{mol}^{-1} \text{m}^3$	$Z \times 10^{-4}$ $\text{Kgm}^{-2}\text{s}^{-1}$
0.1	0.7	1487	0.8431	740.21	6.10	0.513	2.140×10^{-8}	1.10×10^6
0.2	0.6	1421	0.9378	810.31	6.03	0.509	1.830×10^{-8}	1.15×10^6
0.3	0.5	1382	0.9821	848.56	6.17	0.515	1.610×10^{-8}	1.17×10^6
0.4	0.4	1290	1.2834	868.51	6.93	0.546	0.991×10^{-8}	1.12×10^6
0.5	0.3	1249	1.2911	890.11	7.21	0.557	0.878×10^{-8}	1.11×10^6
0.6	0.2	1192	1.3174	911.32	7.72	0.576	0.754×10^{-8}	1.09×10^6
0.7	0.1	1121	1.3419	940.86	8.46	0.603	0.635×10^{-8}	1.05×10^6

The ultrasonic velocity of mixtures decreases gradually as the mole fraction of 1-butanol increases as shown in fig -1. In liquid/gas mixtures, ultrasonic velocity will be greatly affected by intermolecular forces between molecules in the mixture and by the arrangement of the molecules themselves. This reduction in the ultrasonic velocity of the mixture suggests decreasing cohesion forces between the components in the mixture and an increase in the distance between the molecules in the mixture. This type of behavior is indicative of stronger intermolecular forces being disrupted and

weaker intermolecular forces dominating in the binary mixture. Acetylcholine contains polar functional groups capable of forming dipole–dipole interactions while 1-butanol has a hydroxyl group capable of forming hydrogen bonds with other molecules in the mixture. At lower concentrations of 1-butanol, it is possible to have hydrogen bonding between the polar site of acetylcholine and the hydroxyl group of 1-butanol. As the mole fraction of 1-butanol increases, hydrogen bonding will decrease due to molecular rearrangements within the liquid mixture. [11,12]. The Fig-2 shows the how viscosity changes with mole fraction of the binary mixtures. The changes in acoustic impedance provide additional support for this explanation. With increasing mole fraction of 1-butanol, there is an initial small increment of acoustic impedance followed by a continual decrease. As both density and ultrasonic velocity contribute to acoustic impedance, a change in acoustic impedance shows how well molecules are packed within a liquid. The early increase probably occurs from favourable interactions occurring between dissimilar molecules and, therefore, should help bring about a dense packing of molecules due to hydrogen bonding or dipole-dipole forces. Changes in acoustic impedance indicate a continuing decrease in the structural compactness and greater relative importance of weak dispersive forces, as 1-butanol concentration increases. [13]



In addition to changes in acoustic impedance, adiabatic compressibility (β) also increases with increasing mole fraction of 1-butanol, which reflects how tightly packed liquids are. Increased compressibility indicates that the mixture is becoming easier to compress, hence indicating a decrease in relative intermolecular cohesive forces and an increase in relative free volume within the mixture. As ultrasonic velocity is inversely proportional to compressibility, the observed increase in the compressibility of the liquid mixture is in agreement with the observed decrease in ultrasonic velocity. This trend indicates that the arrangements of molecules become less tightly packed with increasing 1-butanol concentrations [14].

1-butanol has a moles-per-mole fraction (an increasing mole fraction) relationship with the intermolecular free length (L_f). The intermolecular free length (L_f) is the statistically average distance that separates neighboring molecules, which is related to the compressibility of the molecule. The growing intermolecular free length (L_f) reinforces the strength of the attractive forces and indicates a much less compact molecular structure of the molecule (1-butanol) at higher concentrations. Several types of free lengths (L_f) exist to define the molecular property of dissolution times. The dissolution times (τ) also have an increasing relationship with increased 1-butanol mole fraction. The dissolution time increases with increased viscosity (increased τ) due to greater resistance to molecular mobility than lower viscosity liquids. The long hydrocarbon group of 1-butanol gives rise to greater dispersion forces between alkyl groups; however, the overall polarity of the 1-butanol molecule remains low. The dominant hydrophobic forces at higher concentrations of 1-butanol cause the non-specific interaction forces (e.g., hydrogen bonds) between the two mixed molecules to weaken. The different molecular properties of 1-butanol show significant structural changes in the two component (liquid) mixtures due to decreased intermolecular attraction forces between the two components with increasing 1-butanol mole fraction.

IV. CONCLUSION

The ultrasonic velocity, density, and viscosity of acetylcholine–1-butanol binary mixtures were measured at 303 K to examine the nature of molecular interactions present in the system. The experimental results show that the ultrasonic velocity decreases with increasing mole fraction of 1-butanol, while both density and viscosity increase; suggesting enhanced molecular association within the mixture. In addition, the calculated adiabatic compressibility and intermolecular free length were found to increase, indicating structural rearrangement and changes in packing between the molecules. Overall, these findings clearly demonstrate the presence of strong intermolecular interactions, primarily governed by hydrogen bonding and dipole–dipole interactions between the components. The study therefore confirms

that the ultrasonic technique is a reliable and effective method for probing molecular interactions and structural behavior in biologically relevant solvent systems.

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