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STUDY OF MOLECULAR INTERACTIONS OF 3, 4-DIHYDROXY-5-NITROBENZALDEHYDE IN ETHANOL USING ULTRASONIC INTERFEROMETER

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ABSTRACT

Density and ultrasonic velocity by interferometer at 2 MHz have been measured for the medicinally important compound 3, 4-dihydroxy-5-nitrobenzaldehyde in ethanol as a solvent at different concentrations at constant temperature 303 K. The data obtained is used to evaluate the different thermodynamic and acoustic properties like adiabatic compressibility, apparent molar compressibility, acoustic impedance, relative association, intermolecular free length etc. From these thermodynamic and acoustic properties, the molecular interactions like solute-solute and solute-solvent occurring in solution have been interpreted, with respect to change in concentration.

Keywords: Ultrasonic interferometer, Adiabatic compressibility, Acoustic, molecular interaction.

INTRODUCTION

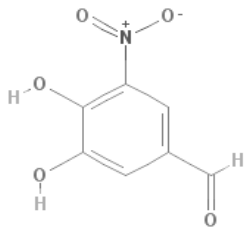
The property of sound wave is that, it gives information about adiabatic properties of the solution. The molecular interaction is useful for understanding physico-chemical behavior of liquid. To study the liquid theory the acoustic properties as ultrasonic velocity, adiabatic compressibility are very useful. The most precise property of sound wave is that it gives information about adiabatic properties of solution. Now-a-days molecular interactions are mostly studied by ultrasonic interferometer[1-3]. It is also useful in understanding physico-chemical behavior of liquids. The structural arrangements are influenced by the shape of the molecules as well as by their mutual interactions.

In view of the medicinal and pharmaceutical significance of 3, 4-dihydroxy-5-nitrobenzaldehyde, we intended to study the intermolecular interactions by ultrasonic interferometer. The solute-solvent molecular interaction was studied by Aswale S. S. *etal* [4-7]. Effect of concentration and temperature on molecular interaction in the solution of drugs can be studied from acoustic and thermodynamic properties. Similar work was carried out from this laboratory [8-10]. An attempt in this investigation is made to study the intermolecular interactions of 3, 4-dihydroxy-5-nitrobenzaldehyde in ethanol with the effect of change in concentration. The acoustic properties like adiabatic compressibility apparent molar compressibility, acoustic impedance, relative association, intermolecular free length etc. are determined from the ultrasonic velocity and density measurements of the solutions at 303K. From the observations of these properties the molecular interactions are predicted.

EXPERIMENTAL

AR grade ethanol was used as a solvent. 3, 4-Dihydroxy-5-nitrobenzaldehyde was obtained from Ramdev Chemical as a gift sample. Density was measured with the help of density bottle. The density of ethanol was measured at 303K. Sample weighing was done on Roy CCB-4 Balance having an accuracy of ±0.001g. Single crystal interferometer (Mittal Enterprises, Model F-81) with accuracy of ± 0.03% and frequency 2 MHz was used in the present work. The working of the ultrasonic interferometer was checked by measuring ultrasonic velocity of pure water at 303K. The measured value 1508 ms^{-1}.which is very close to theoretical[11] value 1515 ms^{-1} and confirms the accuracy of instrument. 0.1M solution of 3, 4-dihydroxy-5-nitrobenzaldehyde was prepared in ethanol at 303K. The densities and ultrasonic velocities

of all solutions were measured at 303K. Similar measurements were carried out for 0.01M and 0.001M solution of 3, 4-dihydroxy-5-nitrobenzaldehyde in ethanol.



3, 4-dihydroxy-5-nitrobenzaldehyde

RESULTS AND DISCUSSION

In the present investigation, measurements of densities and ultrasonic velocities of 3, 4-dihydroxy-5-nitrobenzaldehyde in solvent ethanol at 0.1M, 0.01M and 0.001M concentration at 303 K at 2 MHz frequency have been made, and given in Table 1. The adiabatic compressibility (β) is evaluated by using equation.

$$\beta = 1 / v^2.d \quad (1)$$

Apparent molar compressibility (ϕK) is an acoustic property which is determined by measuring density and ultrasonic velocity and depends upon the molality of solution and molecular weight of the solute, by the relation,

$$\phi K = [1000 (\beta_s d_0 - \beta_0 d_s) / m d_s d_0] + (\beta_s M / d_s) \quad (2)$$

Where, d_0 = density of pure solvent, d_s = density of solution, m = molality of solution, M = molecular weight of solute, β_0 = adiabatic compressibility of pure solvent, and βs = adiabatic compressibility of solution.

Specific acoustic impedance is determined from the measurement of ultrasonic velocity and density by formula,

$$Z = vs. ds \quad (3)$$

The solute-solvent interactions may be interpreted in terms of acoustic impedance. Relative association is a function of ultrasonic velocity and is computed by the equation,

$$RA = d_s/d_0(v_0/v_s)^{1/3} \quad (4)$$

Where, v_0 and v_s are ultrasonic velocities in solvent and solution.

Intermolecular free length (L_f) is one of the important acoustic properties to study the intermolecular interactions. Intermolecular free length has been evaluated from adiabatic compressibility (β) by Jacobson's[12-14] formula,

$$L_f = K.\sqrt{\beta_s} \quad (5)$$

Where, K is the temperature dependent constant known as Jacobson's constant and is independent of the nature of liquid, (At 303.15 K, K=627).

This paper deals with study of molecular interaction of 3, 4-dihydroxy-5-nitrobenzaldehyde in ethanol at 303K. From experimental data we reported ultrasound velocity, and density in this paper. Thermodynamic and acoustic properties like adiabatic compressibility (β), specific acoustic impedance (Z), apparent molar compressibility (ϕK), Relative association (R_A) and intermolecular free length(L_f) are

studied and results are tabulated in Table 1 and graphed at three different concentration levels i.e. 0.1M , 0.01 and 0.001M as Figures 1-6.

From Table-1 it is seen that increase in concentration results in increase in number of particles in given region which leads shrinkage in volume of solution and hence density increases with increase of concentration.

Table-1: Acoustic and thermodynamic parameters for alcoholic solution of 3, 4-Dihydroxy-5-Nitrobenzaldehyde at 2MHz

Concentration (M)	Ultrasonic velocity	Density (Kg/m^3)	Adiabatic compressibility ßx10^{-10}	Apparent molar compressibility (ϕK)	Specific acoustic impedance $Zx10^4$ ($Kgm^{-2}sec^{-1}$)	Relative Association R_A	Intermolecular free length L_f (A^0)
Ethanol	1761.95	779.65	4.1315	-	-	-	-
0.001	1698.37	786.23	4.4094	3.10 x10^{-8}	133.5317	1.024	0.0133
0.01	1465.34	787.12	5.9167	2.23 x10^{-8}	115.3398	1.0471	0.0152
0.1	1420.78	788.03	6.2864	2.82 x10^{-9}	111.9617	0.8543	0.0157

As concentration increases number of molecules in the medium increases, making the medium to be denser, this leads to greater compressibility resulting in slow transfer of sound waves and hence ultrasonic velocity decreases with increase of concentration as shown in Figure-1. This decrease in Ultrasonic velocity with increase in concentration shows less interaction between solute and solvent molecules. It is due to formation of less hydrogen bonding.

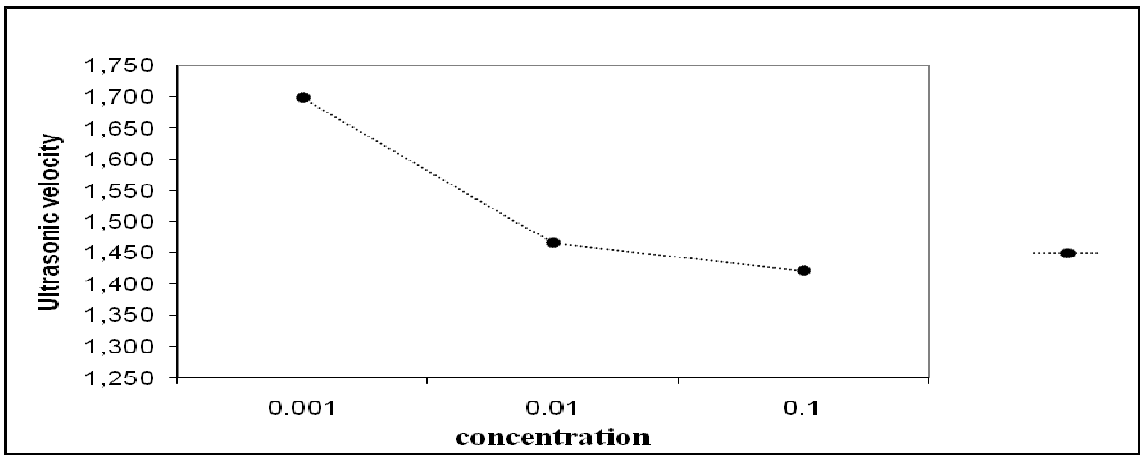


Fig.-1: Ultrasonic velocity at 303k (v) 3, 4-dihydroxy-5-nitrobenzaldehyde

From Figure-2 it is observed that adiabatic compressibility increases with increases in concentration showing that weak interaction exists in the solution. It shows that there is less possibility of formation of hydrogen bond. The variation in adiabatic compressibility is also supported by variation in specific acoustic impedance.

Like adiabatic compressibility (β) apparent molar compressibility (ϕK) is another important acoustic parameter, which explains the solute-solvent and solute-solute interactions in solutions. It not only depends upon density and ultrasonic velocity like β but also the molecular weight of solute and molarity of solution. Thus, the structure of solute will have direct effect on ϕK values. Apparent molar compressibility property is fairly sensitive to structure changes especially in highly structured solvent and is hence expected to throw interesting light[15]. An addition of solute in ethanol solvent may produce weak

interaction of the Vender Wall forces, which is expected to introduce structuredness in the solution. That is specific arrangement of ethanol molecule may be occurring due to attached solute molecules. Figure 3 shows that adiabatic compressibility increases association of molecule by lower β values, whereas, apparent molar compressibility also shows the increased association but at the same time structuredness of the solution by higher ϕK values. It was observed that apparent molar compressibility gets decreased with increase in concentration.

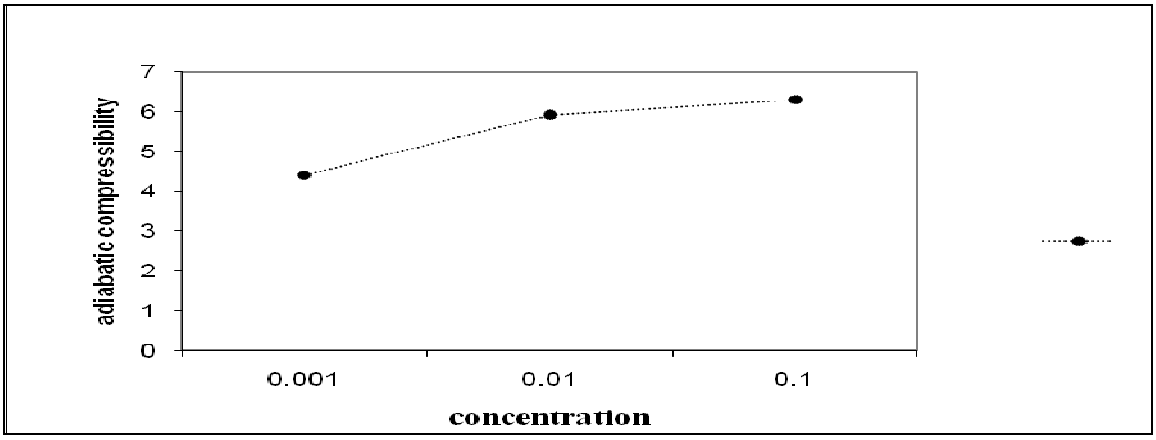


Fig.-2: Adiabatic compressibility (β) 3, 4-dihydroxy-5-nitrobenzalde

Specific acoustic impedance is defined as impedance offered to the sound wave by components of mixture. Mathematically it is directly proportional to ultrasonic velocity and inversely proportional to that of adiabatic compressibility and shows similar behavior to that of ultrasonic velocity and opposite to that of adiabatic compressibility. Specific acoustic impedance also makes the contribution in explaining molecular interactions. Literature shows that the impedance approach to explain the molecular interaction in liquid mixtures has been rather less commonly employed[16]. This is one of the reasons why the impedance approach has been adopted here, to examine the behavior of the solution regarding molecular interactions. The conventional approach based on compressibility is both useful and fundamental; however, acoustic impedance constitutes an additional probe for studying molecular interactions. Specific acoustic impedance is the complex ratio of the effective sound pressure at a point to the effective particle velocity at that point. The Figure-4 explains the above fact that as the concentration increases the specific acoustic impedance decreases.

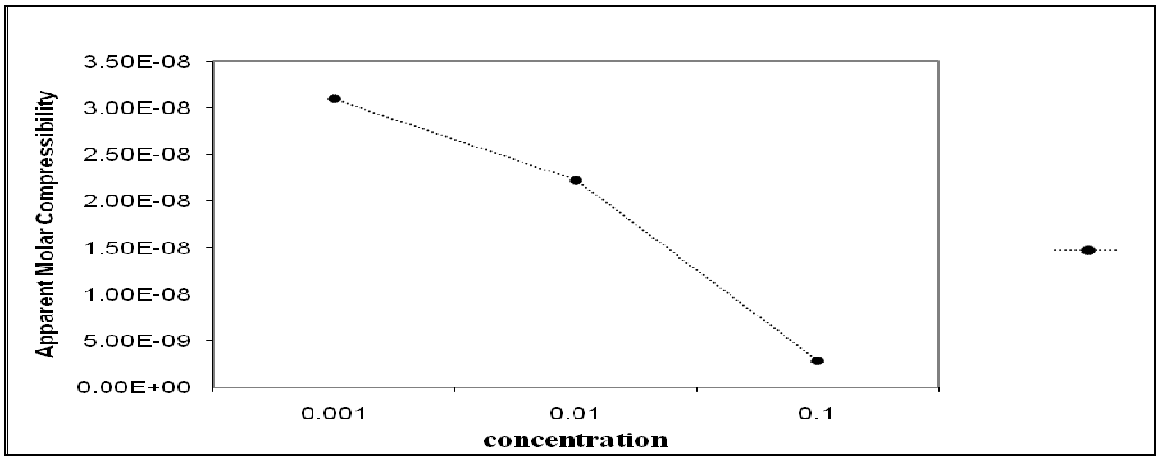


Fig.-3: Apparent molar compressibility of 3, 4-dihydroxy-5-nitrobenzaldehyde

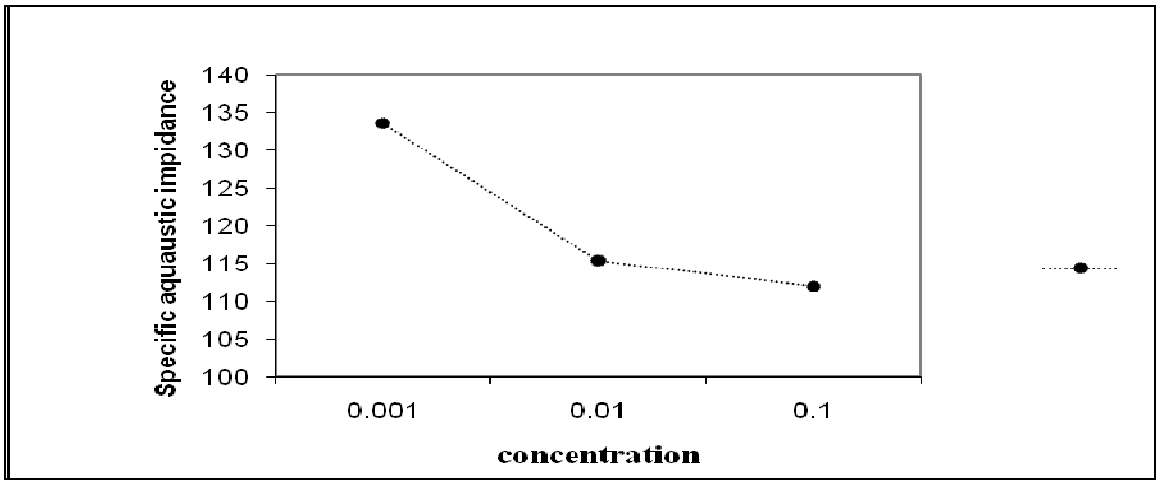


Fig.-4: Specific acoustic impedance of 3, 4-dihydroxy-5-nitrobenzaldehyde

Relative association is an acoustic property of understanding interaction, which is influenced[17] by two opposing factors:

i. Breaking of solvent structure on addition of solute to it and
ii. Salvation of the solutes, those are simultaneously present, by the free solvent molecule.

Relative association as seen in Figure 5 varies non linearly with concentration which reveals that the specific interaction exists in the solution.

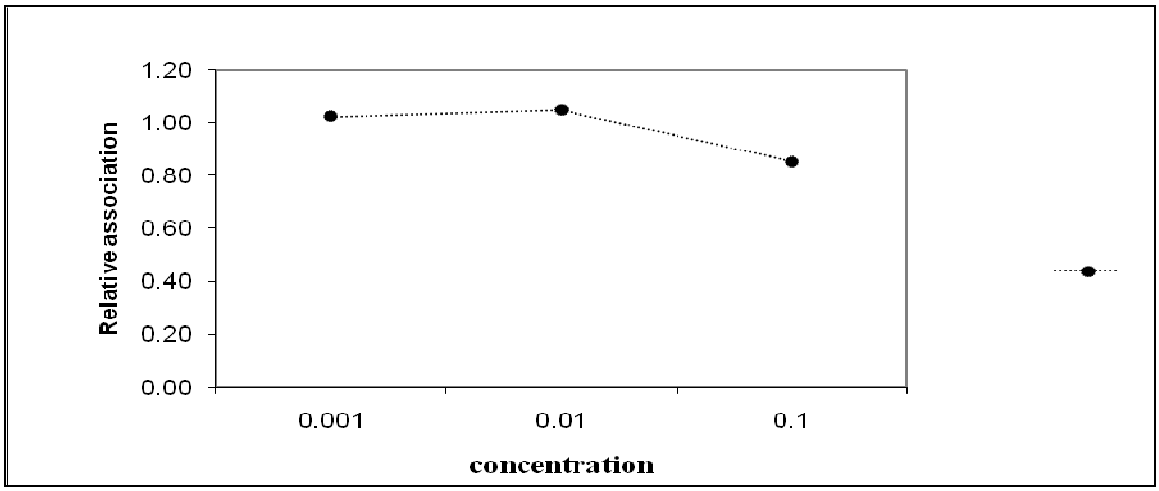


Fig.-5: Relative association of 3, 4-dihydroxy-5-nitrobenzaldehyde

Intermolecular free length is the distance between surfaces of the neighboring molecules. Eyring and Kincaid[17] have proposed that free length is dominant factor in determining the variation of ultrasonic velocity of solution. Ultrasonic velocity depends on intermolecular free length L_f with decrease in free length velocity increases or vice versa. Mathematically intermolecular free length is directly proportional to adiabatic compressibility and inversely proportional to ultrasonic velocity and shows similar behavior to that of adiabatic compressibility and opposite to that of Ultrasonic velocity. As per Figure 6 as free length increases with concentration, the increase in free length shows weak molecular interaction while decrease in free length signifies specific interaction existing in the solution.

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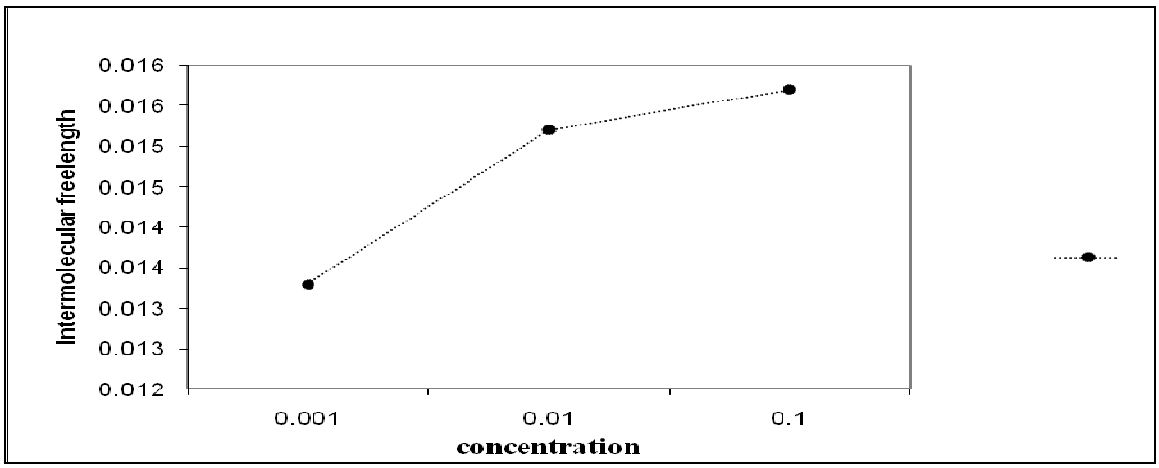

Fig.-6: Intermolecular free length of 3, 4-dihydroxy-5-nitrobenzaldehyde

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