Adiabatic Compressibility, Free Length and Acoustic Impedance of Sodium Benzoate in Ethanol Water Mixtures

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Abstract: — The study of thermodynamic molecular interactions of sodium benzoates in aqueous organic medium gives useful information in industrial chemistry. The study of ultrasonic parameters is directly related to a number of thermodynamic parameters. The ultrasonic velocity, density and viscosity are measured for various solutions of sodium benzoate in ethanol water media. Using the above data the acoustic parameters like adiabatic compressibility, free length and specific acoustic impedance are evaluated. The variation of these parameters gives interesting and useful information regarding the molecular interaction existing in the solution.

Key words: Free length, adiabatic compressibility, molecular interaction, sodium benzoate, ethanol water mixture

I. INTRODUCTION

In recent years, the study of intermolecular interaction in liquid mixtures is vastly studied by ultrasonic techniques [1-3]. This is due to the ability of such techniques delving into the molecular behavior of liquids and solids throwing light on its physiochemical behavior of the medium [4-6]. The measurement of ultrasonic velocity has been consistently used in the field of interactions and structural aspect evaluation studies, especially at the macro level.

Binary mixture studies are indispensable for many chemical processes, including solubility effects, calculation of speciation, phase equilibrium, absorption and distribution of drug and drug products. The study of thermodynamic properties plays a vital role in assessing the compactness due to molecular interaction. These properties have attracted much attention of scientists and experimental data on a number of binary systems are available from review and publication [7-10]. The viscosity, velocity and density measurements derived from these systems depict the solute-solute and solute-solvent interactions.

The present study deals with the study of molecular interaction of sodium benzoate in ethanol-water mixtures at 303K. Sodium Benzoate is the sodium salt of benzoic acid. It is widely used as a preservative, in urea cycle disorders and even in fireworks. Ethanol is a highly protic polar solvent. It is greatly soluble in water and readily forms hydrogen bonds in solution. The molecular interaction studies with alcohol as one of the constituents in binary mixtures is of special interest because alcohols are strongly self associated liquids with a three dimensional network of hydrogen bonds. They can get associated with any other group having similar degree of polar attraction [11, 12]. The data obtained from the ultrasonic propagation parameters in the ethanol solvent media highlights the existence of interaction between the different species in liquid mixtures. The non-linear variation of ultrasonic velocity, compressibility and linear free length are related to the structural changes occurring in a liquid as its concentration is varied.

II. MATERIALS AND METHODS

The chemicals used in the present study were of high purity and analytical grade (E.Merck, India). Purification was done by standard procedure [13-15] and the solvent was redistilled before use. The density of the purified solvent used was 0.7806gcm-3 with a coefficient of viscosity of 0.9590mPa.s at room temperature. The density of the liquids was measured using a10ml specific gravity bottle. The viscosity of the pure liquids and the liquid mixtures were measured using an Oswald's viscometer with an accuracy of 0.01s. Ultrasonic velocity was measured by a single crystal variable path interferometer with an estimated accuracy of ±0.05%. Triply distilled water (specific conductivity of the order of 1×10-7 Scm-1) was used throughout this study.

III. RESULTS AND DISCUSSION

Table 1: Values of Density (ρ), Viscosity (η) and Ultrasonic velocity (U) of 0.001 M Sodium benzoate in ethanol + water at 303 K.

Concentration (M) of Sodium Benzoate	% of Ethanol	Density ρ(Kg/m^3)	Viscosity η(m.Pa.s)	Velocity U(m/s)
0.001	5	0.994	1.045	1546
	10	0.993	1.123	1547
	15	0.992	1.201	1571
	20	0.991	1.474	1604
	25	0.963	1.596	1619
	30	0.953	1.659	1623
	40	0.944	2.0054	1654
	50	0.923	2.208	1554
	60	0.911	2.297	1505
	70	0.896	2.242	1400
	80	0.844	1.988	1323

The experimental values of density, viscosity and ultrasonic velocity of 0.001M Sodium Benzoate in several proportions of ethanol water mixtures ranging from 5% to 80% are given in Table 1.

From the observed values various thermodynamic parameters like adiabatic compressibility, intermolecular free length and the acoustic impedance were calculated. The parameters adiabatic compressibility (β ad), free length Lf, and acoustic impedance at 303K are listed in Table 2.

Table 2: Values of Adiabatic compressibility (β), Intermolecular free length (Lf) and Acoustic impedance of 0.001 M Sodium benzoate in ethanol + water at 303K.

Concentration (M) of Sodium Benzoate	% of Ethanol	Adiabatic Compressibility β X10-7 (m^{2}N^{-1})	Intermolecular free length X105 Lf (A0)	Specific acoustic impedance Z (Kgm^{-2} s^{-1})
0.001	5	4.209	27.76	1536.72
	10	4.207	27.76	1536.17
	15	4.084	27.35	1558.43
	20	3.92	26.79	1589.56
	25	3.96	26.93	1559.09
	30	3.98	27.00	1546.71
	40	3.87	26.62	1561.37
	50	4.48	28.64	1434.34
	60	4.84	29.77	1371.05
	70	5.69	32.28	1254.4
	80	6.76	35.18	1116.61

Adiabatic compressibility (β) has been calculated from the speed of sound and density of the medium using the equation as:

$$\beta = 1/ (u2\rho)$$

where U is the ultrasonic velocity and ρ is the density.

The intermolecular free length (Lf) has been determined using the Jacobson's formula,

$$Lf = K$$

where K is a temperature independent constant called as the Jacobson's constant which is equal to 4.28 X 109 for all liquids.

Specific acoustic impedance (Z) has been calculated by using the equation

$$Z = \rho.U$$

where ρ is the density and U is the ultrasonic velocity.

Figure 1: Density measurements of 0.001M Sodium Benzoate in Ethanol Water system

It is seen from the Table 1 that the densities of the aqueous sodium benzoate solutions decrease with the increase in the percentage of ethanol content in the medium. This is graphically predicted in Figure 1 where the density measurements of 0.001M sodium benzoate are studied as a function of the percentage of ethanol content.

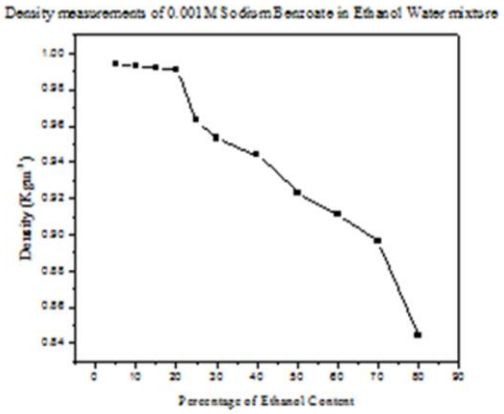

Figure 1: Density measurements of 0.001M Sodium Benzoate in Ethanol Water system The UV absorption spectrum of the synthesized CuGT (Fig3.1) carried out on a JASCO UV Vis shows absorption at 466nm.

It is seen from the figure that the density decreases with the increase of alcohol content. This may be due to the ionic hydration and an increased intermolecular interaction between the ethanol and water molecules complimenting with the similar trend as seen in literature [16 and17]. On mixing ethanol and water the solution gets warmer and there is a minute release in the heat of the solution. The mixture hence becomes less dense on mixing ethanol and water and the specific gravity gets lowered.

The viscosity values of the solutions listed in table 1 reveals the fact that with an increase in the ethanol content the viscosity increases up to 50% and then steadily decreases. The results have been graphically presented in Fig.2.

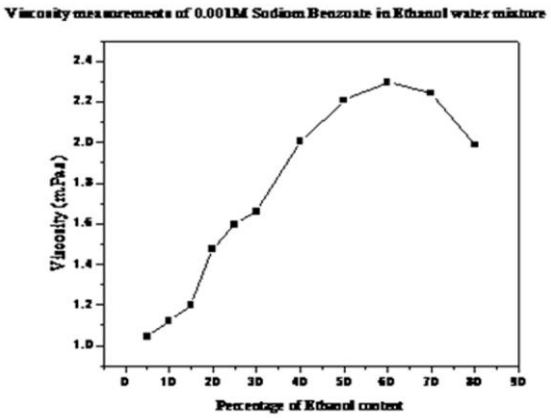

Figure 2: Viscosity measurements of 0.001M Sodium Benzoate in Ethanol Water system

It is seen from the figure that the mobility of ions decreases at 50% to 70% of ethanol in the presence of Sodium benzoate. The water structure is hence expected to be completely broken down, and the mixture indulges in fixing up of maximum energy to activate itself at such a composition [18].

The speed of ultrasonic sound is directly related to the adiabatic compressibility and density. It is seen from Fig.3 and Table 1 that the ultrasonic velocity of sodium benzoate in the aqueous solutions of ethanol initially increases up to 40%, starts decreasing at 50% and steeply decreases up to 80% with the addition of ethanol. When sodium benzoate is dissolved in water the water structure gets disturbed initially. There is then a structural reorganization leaving the molecules in closely fitting helical cavities [19].The close packing of water molecules is due to the increased cohesion in the medium. The ultrasonic velocity of the solutions thus starts increasing with the increase in ethanol content which is due to the ionic hydration and an increased cohesion. It is hence seen at the initial stages, with lower proportions of ethanol the water molecules are attached to the ions by strong electrostatic forces. These forces are responsible for introducing a greater cohesion in the solution. It is hence known that the cohesion increases with an increase in the percentage of ethanol. The water structure is hence enhanced further with an increased electrostriction and association.

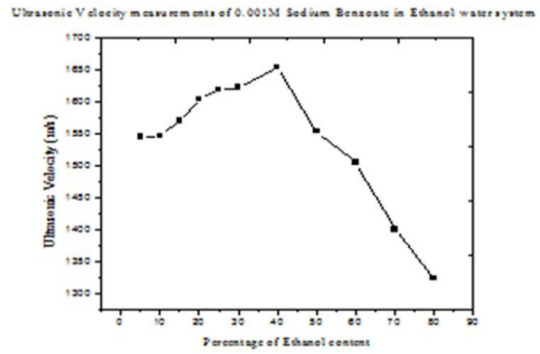

Figure 3: Ultrasonic velocity measurements of 0.001M Sodium Benzoate in Ethanol Water system

Fig. 4 represents the deviation in adiabatic compressibility with the percentage of ethanol content in the binary mixture. The deviation from linearity seen in Table 2 and the figure indicates the presence of strong interaction between the molecules. It is hence concluded that at higher ethanol proportions the difference is size and shape of component molecules lead to a decrease in velocity, followed by an increase in compressibility and intermolecular free length. Thus the closer approach of different molecules leads to a reduction in the compressibility and volume [20].

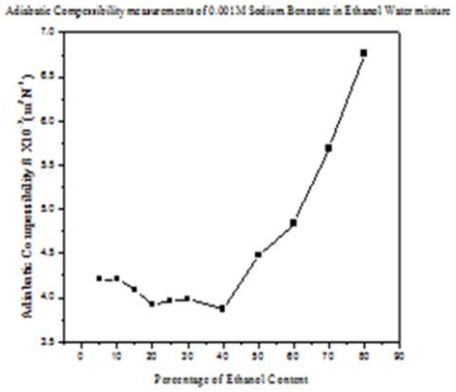

Figure 4: Adiabatic Compressibility measurements of 0.001M Sodium Benzoate in Ethanol Water mixture

The intermolecular free length is considered as the distance between the surfaces of the adjacent molecules. The increase or decrease of the intermolecular free length is directly a result of the variation in ultrasonic velocity of a solution on mixing the several components. On mixing several components the intermolecular free length and adiabatic compressibility are affected. This directly influences the speed of sound. On addition of greater proportions of ethanol, the mixture forms compact molecular aggregates and sound travels faster through the mixture by longitudinal waves. This shows the existence of strong intermolecular interactions highlighting the effect of a strong structure making effect of the binary solvent mixture. This fact is also represented in the present investigation of sodium benzoate in ethanol water mixtures in Table 2 and Figure 5.

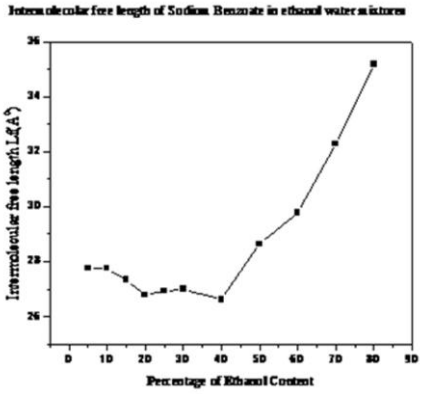

Figure 5: Intermolecular free length measurements of 0.001M Sodium Benzoate in Ethanol water mixtures

Figure 5 represents the variation of intermolecular free length with the percentage of ethanol content. It is seen that the intermolecular free length shows a steep increase at higher ethanol proportions. The dominant nature of interaction between unlike molecules may be attributed to the deviation of Lf values and it is known that the sound wave has to travel a longer distance supporting the data from literature [21].The compressibility nature of solutes is a very sensitive indicator of molecular interactions. It is the second derivative of Gibbs energy and provides useful information about this phenomenon [22-23].

The existence of an electrostatic field between interacting molecules causes structural change of molecules. In addition the change in adiabatic compressibility values in liquids and liquid mixtures is due to the strength of intermolecular attraction. Two effects, namely the electrostatic attraction and the association together predominate and decrease the compressibility of the medium [24].

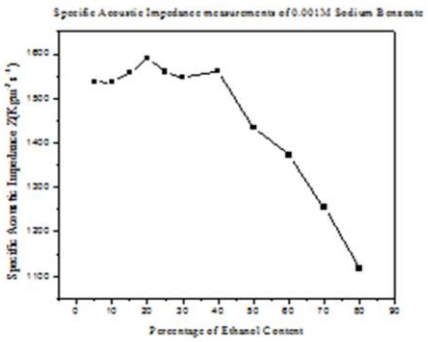

Figure 6: Specific Acoustic Impedance measurements of 0.001M Sodium Benzoate in Ethanol Water mixture

Figure 6 shows the variation of specific acoustic impedance with percentage of ethanol content in the sodium benzoate liquid media. It is known that when an acoustic wave travels in a medium there is a definite pressure variation between the particles. The ratio of the instantaneous excess pressure at any particle to the instantaneous velocity of that particle is called the specific impedance of the medium. The inertial and elastic properties of the medium cause a relative association in the mixture with increase in ethanol content. These results are complimented with the available trend in the literature [3] supporting the possibility of molecular interaction.

The results of adiabatic compressibility βad, Z and Lf thus strengthen the occurrence of strong molecular associations in the binary liquid mixture.

IV. CONCLUSION

The present study probes into the specific role of a mixed solvent in a particular composition of the mixture on the dissociation of sodium benzoate. The intermolecular free length and the adiabatic relationship have an inverse relationship with ultrasonic velocity. The results obtained from the studies of ultrasonic speed, density and viscosity measurements suggest the presence of specific molecular interactions between the molecules of sodium benzoate in several ethanol water mixtures.

V. REFERENCES

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