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Short Communication

Study on Molecular Interactions in Binary Mixture at Variable Frequencies Using Ultrasonic Technique

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Abstract

Densities and ultrasonic speed have been measured at 303K for the binary mixture of di acetone alcohol and Chlorobenzene over entire composition range. From these isentropic compressibility (β), intermolecular free length (L_f), acoustic impedance (Z) and their deviations namely excess isentropic compressibility (β^E), intermolecular free length (L^E_f), acoustic impedance(Z^E)have been calculated and interpreted in terms of intermolecular interactions. Further the variations of these parameters with frequency have been discussed.

Keywords: Binary mixture, ultrasonic speed, isentropic compressibility, acoustic impedance

Introduction

Ultrasonic speed of sound waves in a medium is fundamentally related to the binding forces between the molecules. Ultrasonic speed of the liquid mixtures consisting of polar and polar components are of considerable importance in understanding intermolecular interaction between component molecules and find practical applications in several industrial and technological processes. Variation in thermal and acoustic properties with frequencies provides added information regarding the binary or ternary system [1-7]. The sign and magnitude of the nonlinear deviations from ideality as a function of composition and frequency may be ascribed to the presence of weak or strong type of interaction between unlike molecules. The excess acoustic parameters of binary mixtures have been satisfactorily used in explaining the extent of interactions between mixing components. As a part of our on going research work, the present investigation deals with two important liquids namely Di- Acetone Alcohol (DAA) and chlorobenzene. Both the liquids under investigation are very useful chemicals and of industrial significance. Due to low bioacumalative and readily biodegradable, DAA used as solvent for some liquid paints. It is also used as solvent extrant in purification processes of resin and waxes. It plays a vital role as a component of printing ink in printing industries. The chlorobenzene is mainly used as raw material for synthesis of triphenyl phosphine, phenyls lance and thiophenol.

Theory: The experimental measured values of ultrasonic speed and density are used to compute acoustic parameters such as intermolecular free length (L_f), isentropic compressibility (β), acoustic impedance (Z) and their excess values. The above acoustic parameters are determined with the help of the following relationship.

Isentropic compressibility, $$\beta = \frac{1}{\rho C^2} \quad (1)$$

Intermolecular free length, $$L_f = K\beta^{1/2} \quad (2)$$

Acoustic impedance $$Z = \rho C \quad (3)$$

and their excess values are calculated as

$$\beta^E = \beta_{mix} - (X_A\beta_A + X_B\beta_B) \quad (4)$$

$$L_f{}^E = L_{fmix} - (X_AL_{fA} + X_BL_{fB}) \quad (5)$$

and $$Z^E = Z_{mix} - (X_AZ_A + X_BZ_B) \quad (6)$$

where X_A, X_B,β_A, β_B,β_{mix}, L_{fA}, L_{fB}, L_{fmix} Z_A, Z_B and Z_{mix} are mole fraction, isentropic compressibility ,inter molecular free length and acoustic impedance of chlorobenzene,diacetone and mixture respectively.

Material and Methods

In the present study the chemicals used are of analytical grade purified by standard procedure[8-10] and redistilled before use. Density was determined with a Pyknometer of 25cm^3 capacity, calibrated with de-ionized double distilled water. Ultrasonic speed was measured by a single crystal variable path ultrasonic interferometer model MX-3, Mittal Enterprises New Delhi, India operating at different frequencies of 1MHz, 3MHz and 5MHz. The temperature stability is maintained within 0.1K by circulating thermo stated water around the interferometer cell that contains the liquid, with circulating pump. Binary mixtures of DAA were prepared with chlorobenzene with varying fraction of DAA.

Result and Discussion

Experimentally determined density and ultrasonic speed were used to calculate isentropic compressibility (β), intermolecular free length (L_f), acoustic impedance (Z) and excess values of β^E, L_f^E and Z^E using the standard relations with accuracy up to third decimal digit. The variations of these thermodynamic parameters with entire concentration range of diacetone alcohol at different frequencies for constant temperature are displayed graphically in figure 1 to 4. The figure -1 shows the variation of ultrasonic speed vs mole fraction of diacetone alcohol which is not linear. It is seen that the ultrasonic speed decreases or increases with mole fraction of diacetone alcohol, depending on the ultrasonic speed value of second component. This suggests that dipole-dipole interaction is stronger in pure chlorobenzene for which the ultrasonic speed is high in chlorobenzene rich region for all studied frequencies.

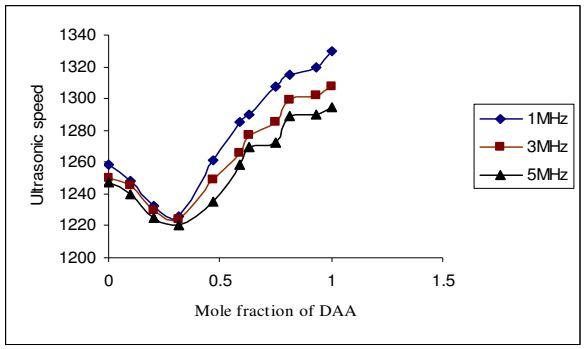

Figure-1
Schematic variation of ultrasonic velocity with mole fraction of DAA

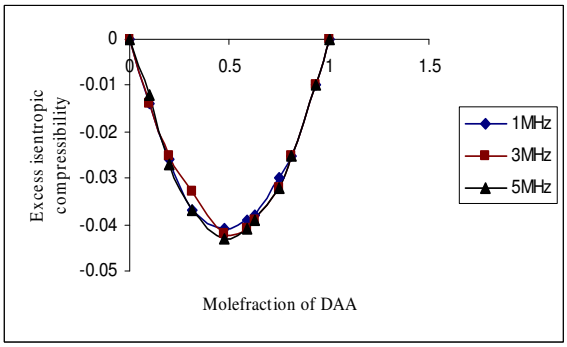

Figure-2
Schematic variation of excess isentropic compressibility mole fraction of DAA

As the concentration of diacetone alcohol gradually increases the different type of interaction comes into existence due to tautomerisim. In diacetone alcohol molecules the hydrogen bonding comes into existence between the like molecules of aldol at –OH end. In addition with hydrogen bonding, keto and enol form of tautomerisim comes into exisistence with maximum percentage of keto form for which the dipole - dipole interaction takes vital role for increasing the ultrasonic speed in high concentration of diacetone alcohol. Considering the effect of frequency it is obvious that, in low concentration of DAA the ultrasonic speed are slightly varies where as in high concentration of DAA the sped increases considerably due to fact that DAA has low density. When frequency increases from 1-5MHz the molecules of the mixture get very less time to interact with each other and they undergoes randomization motion in the medium for which the velocity consequently decreases as compared to low frequency 1MHz. With increase of frequency the enol- form is maximum which leads to formation of maximum amount of H – bonding for which ultrasonic speed decreases with increase of frequency. Figure 2 and 3 demonstrates the variation of β^E and L_f^E for binary mixture of diacetone alcohol and chlorobenzene which are found to be negative over the entire composition range.

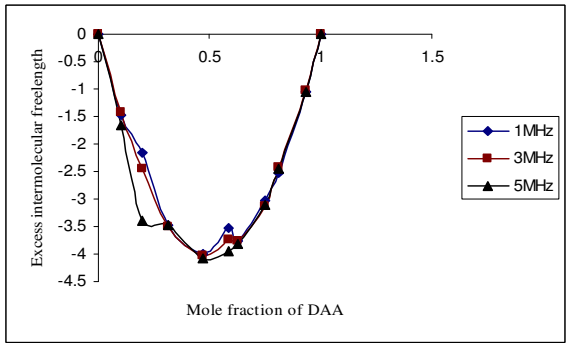

Figure-3
Schematic variation of excess intermolecular free length mole fraction of DAA

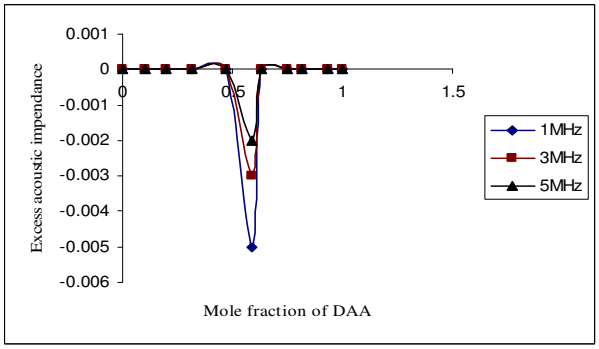

Figure-4
Schematic variation of excess intermolecular free length mole fraction of DAA

Chlorobenzene and diacetone alcohol are being polar liquids; negative values may be interpreted in terms of tautomerism in diacetone alcohol. In enol- form H-bonding occurs among different enol molecules. But the percentage of enol- form is less than keto- form in diacetone alcohol. In keto- form the molecules get associated among themselves in the form of α-multimer. Due to the presence of more keto- form in diacetone alcohol molecule the α -multimer formation will also be more. In pure chlorobenzene only the Vanderwaals interaction is present which a weak interaction. But in a mixture of

chlorobenzene and diacetone alcohol both Vanderwaals interaction as well as multimer formation occurs for which the volume of the mixture may increase. Hence at that point the excess compressibility and excess intermolecular free length will be more. But in pure diacetone alcohol due to strong interaction of α -multimer formation, the volume decreases which decreases the value of β^E and L_f^E for all studied frequencies similar to that of Fort and Moore[11]. Thus it is very clear that with increase of frequency the interaction between the component molecules decreases. The excess value of acoustic impedance (Z^E) is appreciable negative over the entire composition of diacetone alcohol for all frequencies as shown in figure-4. As more than one type of interaction present in a given mixture[12], the increase in mixed interaction like dispersion, H-bonding, α-multimer, dipole-dipole interaction etc. increases the acoustic impedance. The magnitude of Z^E being negative maximum in diacetone alcohol system agrees with the result observed in β^E.

Conclusion

Thus it can be concluded that the interaction of diacetone alcohol with chlorobenzene is stronger in low frequency as is observed in different acoustic parameters for different frequency. The dependence of ultrasonic speed and other derived parameters on composition of the mixture is indicative of the presence of molecular interactions. The sign and magnitude of excess parameter of the mixture and their variations with frequencies reveals that the extent of interaction decreases with increase in frequency.

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