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Research Article

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Ultrasonic Study of Substituted Quinoxaline in Ethanol Solvent at 305.85 K

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ABSTRACT

The density (d) and ultrasonic velocity (v) values have been measured in the solvent ethanol containing 2-hydroxy substituted quinoxaline using different concentration at 305.85 K. The experimental data of density (d), ultrasonic velocity (v), adiabatic compressibility (β), intermolecular free length (L_f), specific acoustic impedance (Z) and relative association (R_A) were calculated. The results obtained in this study have been interpreted in terms of different interactions among solute-solute and solute-solvent.

Keywords: Substituted quinoxaline; Ultrasonic velocity; Density; Acoustic parameter

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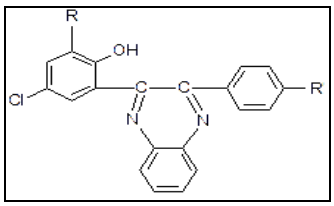
INTRODUCTION

Acoustic parameters were studied to solute-solute and solute-solvent interactions in different solvents. Acoustic parameters provide important and valuable information regarding internal structure, molecular association, complex formation, internal pressure, stability of complexes. In view of analytical, medicinal, agricultural industrial, pharmaceutical significance [1-10]. The variation of ultrasonic velocity and other acoustic parameters along with their excess values in binary and ternary liquid mixtures has been investigated by different authors [11-14]. Ultrasonic study of substituted azomethine drugs in binary mixture [15]. Ultrasonic studies on molecular interaction of benzaldehyde, cinnamaldehyde, 4-methoxy benzaldehyde and diethylamine in n-hexane solutions at 303 K [16]. Molecular interactions in ternary liquid mixture involving toluene at different frequencies [17]. A comparative study of excess Gibb's free energy function values in three binary liquid mixtures containing quinoline and o, m, p-xylenes at different temperatures 303.15, 308.15, 313.15 and 318.15 K [18]. Ultrasonic and volumetric study of aqueous solution of ethylene glycol, propylene glycol in iso-propanol [19]. Viscometric study of carboxymethyl phenol formaldehyde resins in 1,4-dioxane solvent [20]. Volumetric study of strong electrolyte - metal chlorides and metal sulphate in aqueous medium at different temperatures [21]. Volumetric, viscometric and derived surface tension studies on the solutions of potassium dichromate and potassium pyrophosphate in aqueous sorbitol solutions [22]. Study of some important acoustical parameters of substituted-N, N'-bis(salicyliden)-arylmethanediamines in 60% DMF-water at 300 K [23].
Study of thermodynamic properties of Chloline chloride urea in aqueous media at different temperatures [24]. Excess Gibb's free energy function values at different temperatures in binary liquid mixture for the study of molecular interactions [25]. For the present work we have chosen the ultrasonic interferometric technique in order to discuss intermolecular interactions. It is of interest to investigate the acoustic parameters such as adiabatic compressibility (β), intermolecular free length (L_f), specific acoustic impedance (z) and relative association (R_A) of substituted quinoxaline in ethanol solvent at different concentrations of ligand. The different substituted quinoxaline ligand used for present work as:
1) 2-(2-Hydroxy-5-chloro)-benzyl-3-phenyl quinoxaline (L_1)
2) 2-(2-Hydroxy-5-chloro)-benzyl-3-(4-methoxy phenyl) quinoxaline (L_2)
3) 2-(2-Hydroxy-3-bromo-5-chloro)-benzyl-3-phenyl quinoxaline (L_3)
4) 2-(2-Hydroxy-3-bromo-5-chloro)-benzyl-3-(4-methoxy phenyl) quinoxaline (L_4)



R = H or Br; R' = –OCH_3 or H

EXPERIMENTAL SECTION

All the chemicals of A.R. grade were used. Ethanol was purified by described method [25]. Densities were measured with the help of bicapillary Pyknometer with different concentration solution of ligand in ethanol solvent were prepared separately, that weighed on Mechaniki Zaktady Precynynei Gdansk balance made in Poland (±0.001 g). A special thermostatic arrangement was done for density and ultrasonic velocity measurements. Elite thermostatic water bath was used; in which continuous stirring of water was carried out with the help of electric stirrer and temperature variation was maintained within ±0.1°C. Single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy of ±0.03% and frequency 1 MHz was used in the present work. The densities and ultrasonic velocity of ligands in ethanol solvent were measured at 305.85 K.

Calculation

In the present investigation, measurements of densities and ultrasonic velocities of L_1 to L_4 were carried out on ethanol.

Ultrasonic parameters:

Parameters are being extensively used to study molecular interaction in pure liquid [26], liquid mixture [27] and electrolytic solutions [28].

The Adiabatic compressibility (β) can be evaluated by using Laplace's equation.

$$\beta = \frac{1}{v^2.d} \quad \text{……. (1)}$$

Intermolecular free length (L_f) = $K.\sqrt{\beta s}$ ……. (2)

Relative association (R_A) = $\frac{d_s}{d_0}\left[\frac{v_0}{vs}\right]^{1/3}$ ……. (3)

Specific acoustic impedance (z) = $v_s \, . \, d_s$ ……. (4)

RESULTS AND DISCUSSION

The experimentally measured values and calculated values of acoustical parameters such as Density (d), Ultrasonic Velocity (v), Adiabatic Compressibility (β_s), Relative Association (R_A), Intermolecular Free Length (L_f) and Specific Acoustic Impedance (Z) for the ligands (L_1-L_4) are reported in Table 1. The graphs are plotted for Density (d), Ultrasonic Velocity (v), Adiabatic Compressibility (β_s), Relative Association (R_A), Intermolecular Free Length (L_f) and Specific Acoustic Impedance (Z) in various concentrations are shown in Figures 1-6.

Table 1: Acoustic parameters for ligands (L_1-L_4) in ethanol at 305.85 K [Freq=1 MHz]

Ultrasonic Velocity (v)(m sec^{-1})	Adiabatic Compressibility (b × 10^{-6})(pa^{-1})	Relative Association (R_A)	Inter-molecular Free Length (L_f) (A°)	Specific Acoustic Impedance (Z)($kgm^{-2}sec^{-1}$)
347.8	8.4	1.0287	1.8433	338.5485
412	6	0.9688	1.5579	399.64
429.08	5.6	0.9555	1.505	416.0844
449.52	5.1	0.9312	1.4363	431.4493
339.91	8.8	1.0407	1.8867	332.1951
376.48	7.2	1.0034	1.7066	367.0303
399.48	6.4	1.0249	1.609	388.0604
464.72	4.8	0.9252	1.3934	448.1295
345.69	8.5	1.0328	1.8542	337.1503
399.5	6.4	0.9825	1.609	388.9931
436.51	5.4	0.9513	1.4779	423.8553
454.23	4.9	0.9377	1.4078	440.5562
382.5	7	0.9969	1.6827	372.4402
428.46	5.6	0.9556	1.505	415.3035
494.34	4.3	0.892	1.3188	469.1306
592	2.9	0.8502	1.0831	568.6752

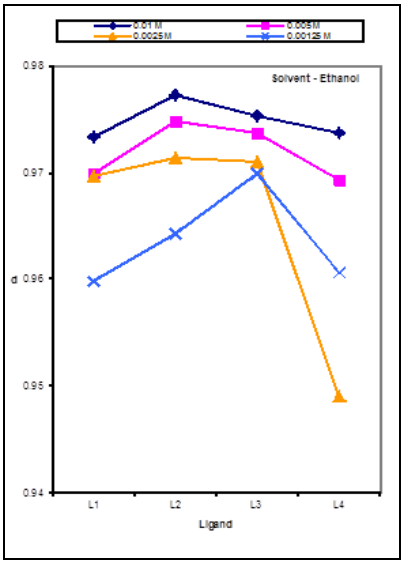


Figure 1: Density of L1, L2, L3 and L4

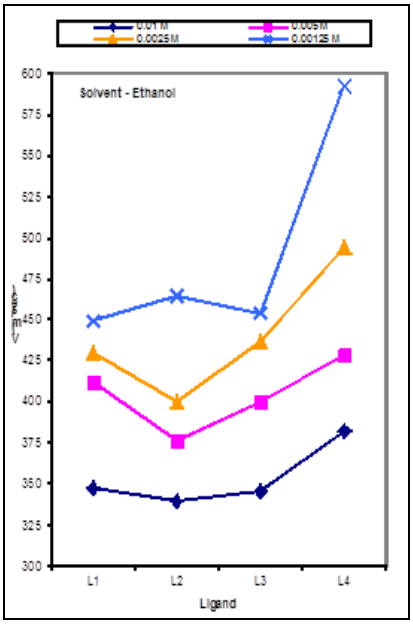


Figure 2: Ultrasonic Velocity of L1, L2, L3 and L4

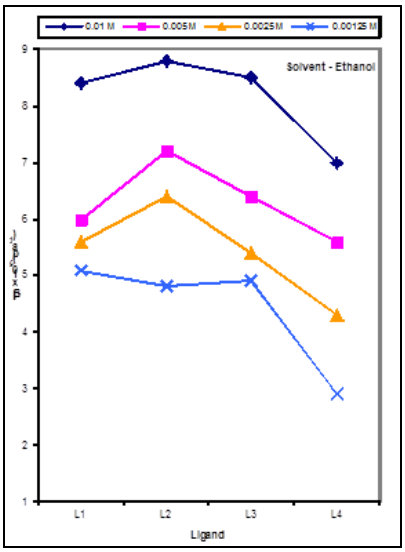


Figure 3: Adiabatic compressibility of L1, L2, L3 and L4

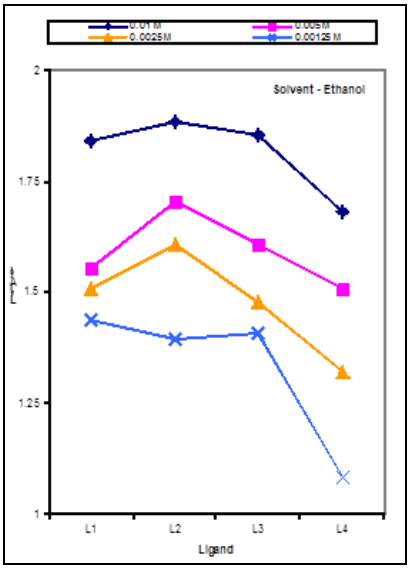


Figure 4: Intermolecular free length of L1, L2, L3 and L4

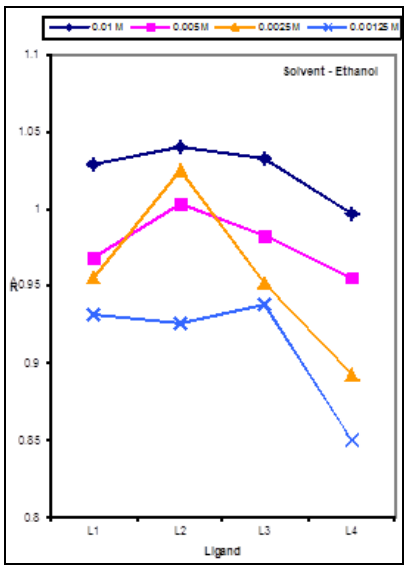


Figure 5: Relative association of L1, L2, L3 and L4

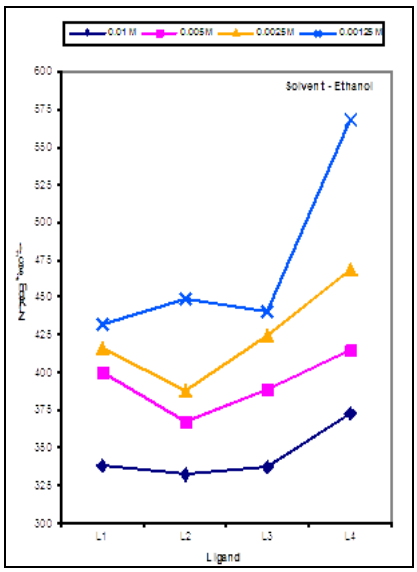


Figure 6: Specific acoustic impedance of L1, L2, L3 and L4

Density is a measure of solvent-solvent and ion-solvent interactions. It is observed that for all ligands L_2 have greater densities than L_3, L_4 and L_1, due to presence of −OH, −Cl, −Br groups. Shows -I effect and +R effect of which latter predominates +R effect increases the electron density. Ultrasonic velocity increases with decrease in concentration. From Figure 2, it was noted that in ethanol L_4 ligand has greater velocity than L_1, L_3 and L_2. Ligand L_4 has higher velocity due to presence of chlorine atom. Chlorine atom has more nucleophillic in nature. Adiabatic compressibility is the important property to study of solute-solvent interactions. The values of adiabatic compressibility are higher for ligand L_2 than L_3, L_1 and L_4. The higher values of β for ligand L_2 and L_3 may be due to the presence of chloro and bromo group in structure. Intermolecular free length for these studies is chosen because, intermolecular forces, which determine the property of liquids, consist of attractive and repulsive forces. The attractive forces depend on the distance between the centers of attraction of molecules, while the repulsive forces are dependent on the distance between the surfaces of molecules. L_2 Ligand has higher intermolecular free length than L_3, L_1 and L_4. Relative association is an acoustic property of understanding interaction which is influenced [29] by two opposing factors; breaking of solvent structure on addition of solute to it and solvation of the solutes that are simultaneously present by the free solvent molecules. The former effect results in the decrease in R_A values while the latter resulting in increase of R_A values. The alcohol molecules are well known to be associated due to hydrogen bonding. The Z values in ethanol are lower indicating hydrogen bonding. The specific acoustic impedance depends upon the various structures of the liquid and the molecular packing in the medium.

CONCLUSION

Acoustic properties such as β, L_f, R_A and z are determined which explain how these interactions occur and responsible for breaking and making of the structure in the solution. So in the present work these acoustic parameters were studied for newly synthesized ligands, which are used as solutes. Density and velocity are determined which explain ion-solvent, solvent-solvent and solute-solvent and molecular interactions in the solution. So in the present work these densities and velocities were studied for synthesized ligands, which are used as solutes using ethanol at temperature 305.85 K in different concentration. The above two studied properties of solvent and solute are not the only prime factors which influence the interactions but the properties of ligand viz. resonance stability of ligand, size of ligand, structure of ligand, heterocyclic nature of ligand and different substituents like electron donating/withdrawing groups in ligands also will have influence on interactions.

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