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Research Article

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Ultrasonic Behaviour and Study of Molecular Interaction of Hydroxy Substituted Quinoxaline in Dioxane Medium

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ABSTRACT

Density (d) and ultrasonic velocity (v) of 2-hydroxy substituted quinoxaline in dioxane were measured at 305.85 K temperature by using ultrasonic interferometer at a frequency of 1 MHz. The study was carried out with change in concentrations. Various thermodynamic parameters such as adiabatic compressibility (β), intermolecular free length (L_f), specific acoustic impedance (Z) and relative association (R_A) were calculated. The results were used to discuss the interaction between solute and solvent. The results are interpreted in terms of molecular interactions like solvent-solvent, solvent-solute and solute-solute.

Keywords: Ultrasonic velocity; Density substituted quinoxaline

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INTRODUCTION

The molecular interaction technique plays a great role for the detection of molecular association, complex formation, internal pressure etc. Ultrasonic is the technique used for the study of molecular interaction in liquids. The structural arrangements are influenced by the shape of the molecules as well as by their mutual interactions. Studies of some ultrasonic parameters of substituted Schiff base in dimethyl formide and ethanol at different temperature [1]. Ultrasonic studies on molecular interactions of $ZnSO_4$ in aqueous solutions of glucose at various concentrations [2]. Molecular interactions in non-electrolyte binary liquid mixtures of cyclohexanol with 2-nitrotoluene and 3-nitrotoluene at four different temperatures [3] and Ultrasonic study of molecular dynamics in some binary mixtures [4]. Ultrasonic studies of molecular interactions of certain zinc electrolytes in poly (ethyleneglycol) [5]. The study of thermophysical properties of binary liquid mixtures of 2-(2-methoxy ethoxy) ethanol (methyl carbitol) with n-butyl amine, sec-butyl amine, tert-butyl amine, n-hexyl amine, n-octyl amine and cyclo hexyl amine at 308.15 K [6] and molecular interaction studies on pharmaceutical drug of 2-[1-(aminomethyl) cyclohexyl] acetic acid in water of various concentrations at 303 K [7]. In view of the analytical, medicinal, agricultural, industrial, pharmaceutical significance [8-12], 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) in dioxane solvent respectively. For the present work we have chosen the ultrasonic interferometric technique in order to discuss intermolecular interactions. From the literature survey it was seen that much work has been done on water and organic solvent mixtures [13-18]. But scanty work is found in pure dioxane solvent. Also the review does not reveal any attempt made on ultrasonic interferometric study of 2-hydroxy substituted quinoxaline.

EXPERIMENTAL SECTION

All the chemicals used were of A.R. grade. 1,4-Dioxane were purified by described method [19]. Densities were measured with the help of bicapillary Pyknometer with different concentration solution of ligand in dioxane solvent were prepared separately, that weighed on Mechaniki Zaktady Precynynei Gdansk balance made in Poland (± 0.001

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 dioxane 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 dioxane.

Density measurement:

The solution was filled in Pyknometer. It was kept in thermostat for 15-20 minutes. It was weighed after checking liquid level in it. Weight of solution was found out by deducting weight of empty Pyknometer from weight of Pyknometer filled with solution using the weight of solution and volume of Pyknometer, density of solution was calculated and average of three density value was considered in calculations.

Ultrasonic parameters:

Parameters are being extensively used to study molecular interaction in pure liquid [20-22], Liquid mixture [23-25] and electrolyte solutions [26].

Ultrasonic velocity and related parameters are:

1. Adiabatic compressibility (β):

By measuring ultrasonic velocity (v) and density (d) experimentally the adiabatic compressibility (β) can be evaluated by using Laplace's equation.

$$\beta = \frac{1}{v^2.d}$$

2. Intermolecular free length (L_f):

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) [27,28] formula:

$$L_f = K.\sqrt{\beta s}$$

3. Relative association (R_A):

Relative association is a function of ultrasonic velocity and is computed by the equation:

$$R_A = \frac{d_s}{d_0}\left[\frac{v_0}{vs}\right]^{1/3}$$

4. Specific acoustic impedance (z):

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

$$z = v_s \,.\, d_s$$

The solute-solvent interactions may be interpreted in terms of acoustic impedance.

RESULTS AND DISCUSSION

In the present investigation density of an ultrasonic velocity measurements have been carried out for the solutions of ligand at different concentrations in dioxane medium. From these values all acoustic parameters such as adiabatic compressibility (β), intermolecular free length (L_f), relative association (R_A) and specific acoustic impedance (z) were determined.

These acoustic properties directly reflects the structural interaction of solvent with solute i.e. ligands at different concentration in dioxane medium and provide important and valuable information regarding internal structure, molecular association, complex formation, internal pressure, stability of complexes. Weak molecular interactions can also be detected by this technique.

These acoustic parameters have been used to investigate the solute-solvent interactions of the ligand at different concentration in dioxane medium. This is serial dilution method and ligands used are -

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)

The acoustic parameters obtained for ligands L_1, L_2, L_3 and L_4 in dioxane solvent at different concentration have been studied to investigate the solute-solute and solute-solvent interactions and the effect of different substituents in the same solvent i.e. dioxane and the effect of dilution on ligand solution.

The experimentally measured values of ultrasonic velocity (v), density (d) and acoustical parameters such as adiabatic compressibility (β), intermolecular free length (L_f), relative association (R_A) and specific acoustic impedance (z) are reported in Table 1 and the graphs were plotted by taking all ligands on X-axis and the value of each property on Y-axis. In the set of graph L_1, L_2, L_3 and L_4 with acoustic properties *viz.* β, L_f, R_A and z are represented in graph (Figures 1-6).

Table 1: Acoustic parameters for ligands in Dioxane at 305.85 K [Freq.=1 MHz]

Ligand	Conc.	v (m sec^{-1})	d (kg m^{-3})	β x 10^{-6} (pa^{-1})	R_A	L_f (A°)	Z ($kgm^{-2}sec^{-1}$)
L_1	0.01	622.13	1.0478	2.4	0.9871	0.9853	651.8713
	0.005	565.56	1.033	3	1.0048	1.1016	584.2235
	0.0025	553.12	1.0266	3.1	1.0058	1.1198	567.833
	0.00125	510.52	1.0227	3.7	1.0291	1.2234	522.1029
L_2	0.01	640.08	1.0482	2.3	0.9781	0.9645	670.9318
	0.005	628.46	1.0335	2.4	0.9703	0.9853	649.5104
	0.0025	563.11	1.0314	3	1.0045	1.1016	580.7928
	0.00125	529.78	1.0233	3.4	1.017	1.1727	542.1215
L_3	0.01	599.47	1.0414	2.6	0.9933	1.0255	624.2845
	0.005	530.15	1.0233	3.4	1.0168	1.1727	542.5025
	0.0025	498.34	1.0223	3.9	1.037	1.256	509.4558
	0.00125	494.48	1.0204	4	1.0377	1.272	504.5732
L_4	0.01	882.08	1.033	1.2	0.8662	0.6967	911.1886
	0.005	674.11	1.0303	2.1	0.945	0.9216	694.5399
	0.0025	662.62	1.0249	2.2	0.9454	0.9433	679.1192
	0.00125	537.87	1.0217	3.3	1.0103	1.1553	549.5383

Density is a measure of solvent-solvent and ion-solvent interactions. It is observed that for all ligands L_2 have greater density than L_1, L_3 and L_4, due to presence of −OH, −Cl, −Br groups, these groups show -I effect and +R effect of which latter predominates +R effect increases the electron density.

Velocity decreases with decrease in concentration. L_4 ligand has greater velocity than L_2, L_1 and L_3. There is also presence of −Cl, −Br and −OH atom. The presence of −Br atom which is bigger in size, -I effect of −Cl are acting on the ligand so this L_4 ligand has highest dipole moment.

Adiabatic compressibility is one of the important properties during the study of solute-solvent interactions and represented byβ. From Figure 3, it can be noted that in dioxane L_3 ligand has higher adiabatic compressibility value than L_1, L_2 and L_4. Ligand L_3 possess chlorine atom -I effect of Cl are acting in ligand. In the present investigation it was noted that the nature of ring structure, total numbers of different atoms present in the ring, resonance stabilization in the ring, total number of electron loan pairs present on hetero atoms, electron donating and electron attracting substituents present nearer to the $-OCH_3$ group on the ligand will directly interfere the interaction between solute and solvent and show change in adiabatic compressibility.

Jacobson pointed out that certain properties of liquid state could be studied to an advantage as a function of free length between molecules. Ligand L_3 has higher intermolecular free length than L_1, L_2 and L_4, because of its non-polar nature. Ultrasonic velocity depends on intermolecular free length L_f. With decrease in free length velocity increases or vice versa.

Relative association is an acoustic property of understanding interaction, which is influenced [29] by two opposing factors;

i) Breaking of solvent structure on addition of solute to it and,
ii) Solvation of the solutes those 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. Specific acoustic impedance is the complex ratio of the effective sound pressure at a point to the effective particle velocity at that point [30]. From Figure 6, the values of z are continuously decreasing on changing the structures of ligands (L_1 to L_4). The specific acoustic impedance depends upon the various structures of the ligand and the molecular packing in the medium.

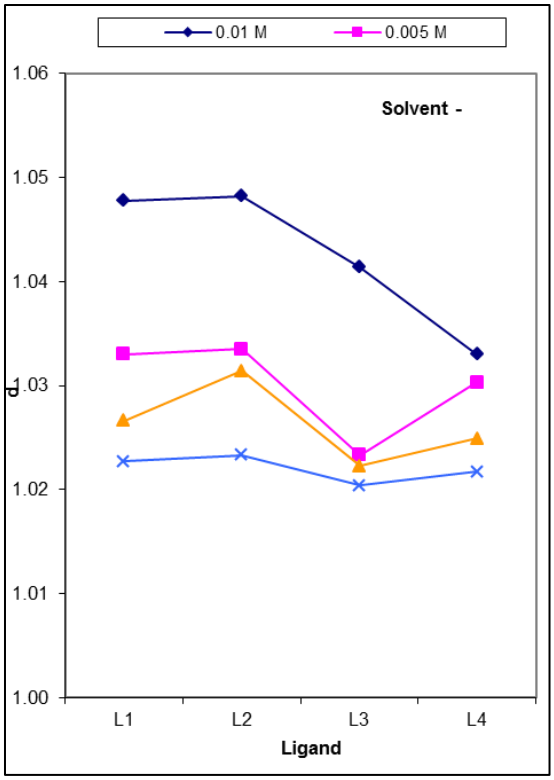

Figure 1: Density of L_1, L_2, L_3 and L_4

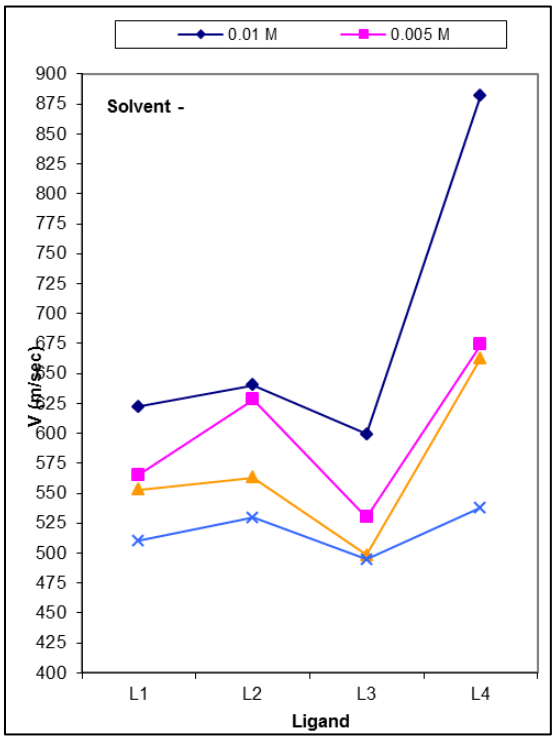

Figure 2: Ultrasonic velocity of L_1, L_2, L_3 and L_4

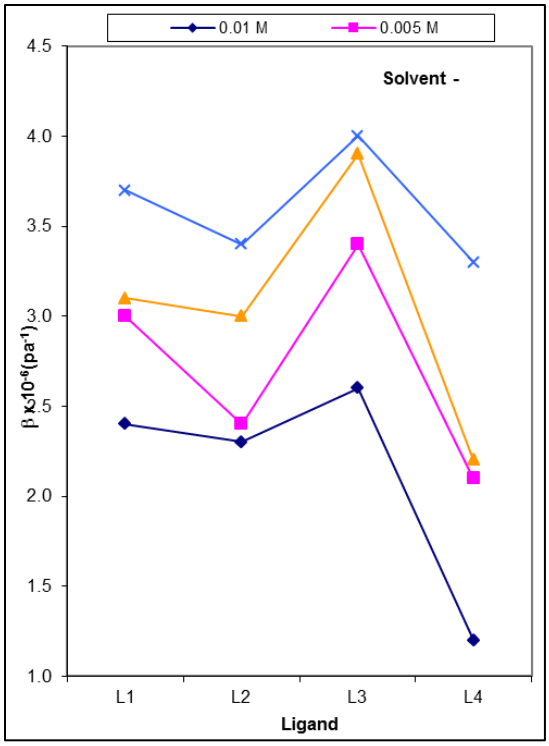

Figure 3: Adiabatic compressibility of L_1, L_2, L_3 and L_4

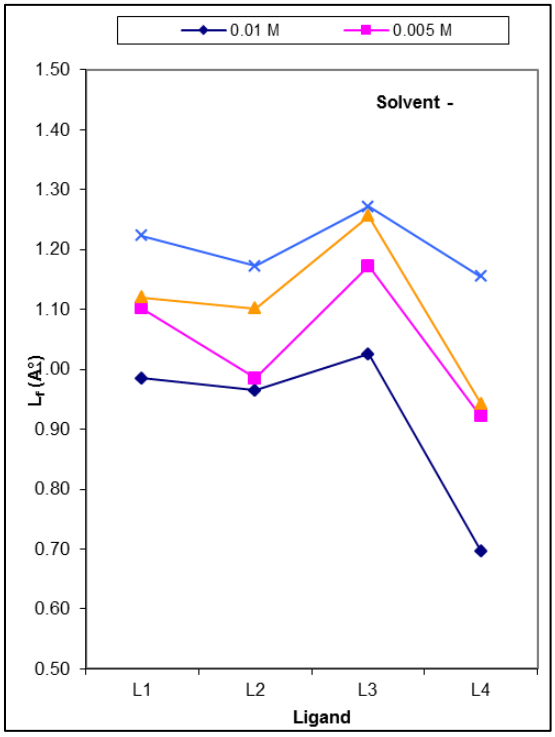

Figure 4: Intermolecular free length of L_1, L_2, L_3 and L_4

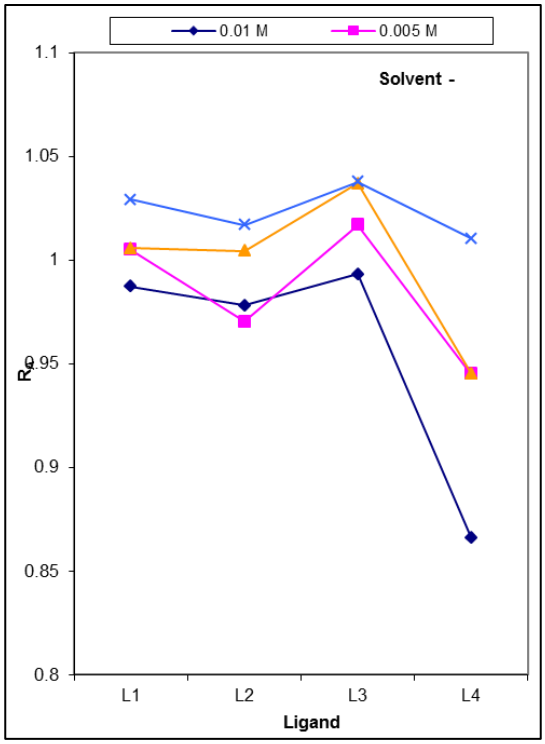

Figure 5: Relative association of L_1, L_2, L_3 and L_4

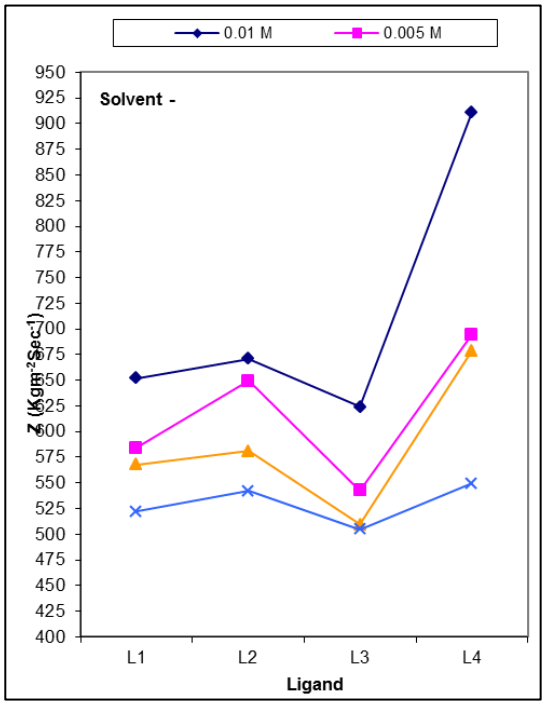

Figure 6: Specific acoustic impedance of L_1, L_2, L_3 and L_4

CONCLUSION

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 1,4-dioxane 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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