Ultrasonic Interferometric Investigation of 2-Hydroxy substituted quinoxaline in Dioxane Medium

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Abstract : Ultrasonic velocity and density measurements of ligand 2-hydroxy substituted quinoxaline were carried out at different concentration in dioxane solvent. For investigating solute-solvent, solute-solute interactions at temperature 305.85 K. The data obtained during the study is used for determining most significant acoustic parameters like velocity (v), density (d), adiabatic compressibility (β), apparent molar volume (ϕ_v), apparent molar compressibility (ϕ_k). The parameters explore solute-solute and solute-solvent interactions in different solvents. In this investigation, the comparative study of effect of solvent and effect of substituents in the solute are studied on molecular interaction of the matter.

Keywords: - Substituted quinaxoline, Acoustic parameters, Interferometry, Solute-solvent interaction.

Introduction

Ultrasonic behavior and study of molecular interaction synthesized Schiff base ligand in different percentage of ethanol-water mixture.[1]Determination of density,ultrasonic velocity and other acoustic parameters of aqueous binary mixtures of substituted hydrazone at 298 K.[2] Acoustic studies on binary liquid mixtures of o-chlorotoulene and ethanol at 303.15K to 318.15K.[3] Adiabatic compressibility,apparent molal volume,apparent molal compressibility and salvation number of 2,3-dihydroquinazolin-4(1H)-one derivatives in 70% DMF-water.[4] Apparent molal volume and viscometric study of ammonium sulphate in 10% DMF-water at temperature 303.15 and 313.15K.[5] Comparative study of intermolecular interactions of S-Triazine and Triazinothio-Carbamides by ultrasonic interferometric technique.[6] Viscometric studies of divalent trasition metal sulphates in mixtures of water-Diethylene glycol at 298.15-318.15K.[7] Solute-Solvent interactions in solutions of 2-hydroxy-5-chloro-3-nitroacetophenone Isonicotinoyhydrazone in N,N-dimethyl-formamide at 298-313K.[8] Experimental and theoretical study of ultrasonic velocity in binary liquid mixture of choloroform and methanol..[9] Ultrasonic interferometric investigations of substituted flavones in aqueous ethanol medium at 301k. .[10] Physico-chemical and excess thermodynamic properties of Acrolein with methanol at 298K temperature and 10MHZ frequency.[11] Study of molecular interactions in antihistamine drug cinnarizine and benzene at different temperatures.[12] Viscometric and thermodynamic study of substituted-N,N'bis(salicyliden) arylmethanediamine in a binary system of 70% DMF-water.[13]Ultrasonic behavior and study of molecular interaction of substituted 3,5-diaryl isoxazoline in 70% DMF-water mixture at 32^0C[14].The use of ultrasound is one of the well recognized approaches for the study of molecular interactions in fluids. The ultrasonic velocity plays an important role in the investigation of intermolecular interactions. Weak molecular interactions can also be studied by ultrasonic technique. The structural arrangement are influenced by the shape of the molecules as well as mutual interactions. The ultrasonic velocity and other acoustic parameters can be measured with great accuracy and consequently provides a powerful way to determine intermolecular interactions.

Hence in this present investigation attempt is made to understand behaviour of substituted

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 ultrasonic velocity and densities of different concentration in dioxane solvent of L_1, L_2, L_3 and L_4 were determined from these β, ϕ_v, ϕ_k were calculated.

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. Different concentration in dioxane 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 L_1, L_2, L_3 and L_4 in dioxane solvent were measured at 305.85 K.

Results and Discussion

A study of β, ϕ_v and ϕ_k directly relate the structural interaction of solvent with solute and provides the information regarding complex formation, stability, internal structure, molecular association and internal pressure. The values of acoustic parameters are given in Table-1.

Density (d)

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.

Ultrasonic velocity (v)

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.

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

Ligand	Conc.	v ($m\ sec^{-1}$)	d ($kg\ m^{-3}$)	$\beta \times 10^{-6}$ (pa^{-1})	ϕ_k ($m^3mol^{-1}pa^{-1}$)	$\phi_v \times 10^3$ (m^3mol^{-1})
L_1	0.01	622.13	1.0478	2.4	-0.1767	-5.7431
	0.005	565.56	1.0330	3.0	-0.2158	-8.6159
	0.0025	553.12	1.0266	3.1	-0.3796	-14.8545
	0.00125	510.52	1.0227	3.7	-0.2585	-26.7735
L_2	0.01	640.08	1.0482	2.3	-0.1871	-5.7870
	0.005	628.46	1.0335	2.4	-0.3378	-8.6936
	0.0025	563.11	1.0314	3.0	-0.4294	-16.857
	0.00125	529.78	1.0233	3.4	-0.5070	-27.2482
L_3	0.01	599.47	1.0414	2.6	-0.1524	-5.0447
	0.005	530.15	1.0233	3.4	-0.1226	-6.4878
	0.0025	498.34	1.0223	3.9	-0.5059	-12.9729
	0.00125	494.48	1.0204	4.0	-0.0167	-24.7772
L_4	0.01	882.08	1.0330	1.2	-0.2898	-4.0348
	0.005	674.11	1.0303	2.1	-0.3947	-7.9356
	0.0025	662.62	1.0249	2.2	-0.7374	-14.0332
	0.00125	537.87	1.0217	3.3	-0.5809	-25.8316

Adiabatic compressibility (β)

It is one of the important properties during the study of solute-solvent interactions. 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.

Apparent molar compressibility (ϕ_k)

The structure of solute and the number of atoms present in it will have direct effect on ϕ_k values. ϕ_k values are negative for all composition of dioxane. This interpret in terms of loss of compressibility of solute due to strong electrostatic salvation of ions. This weak interaction of the Vander Wall forces is expected to introduce structurdness in the solution i.e. specific arrangement of dioxane molecule may be occurring due to attached solute molecules. These spaces may be created making the solution more compressible as it appears from the higher apparent molar compressibility values in dioxane solvent.

Apparent molar volume (ϕ_v)

Apparent molar volume is the thermodynamic property of solutions, which express the solute-solvent interaction is there as oxygen in dioxane also possess negative charge. It results in increase in ϕ_v as the percentage of dioxane in ligand solution increases. L_4 ligand have greater ϕ_v values than L_3, L_1 and L_2.

Fig. 1 : Density of L_1, L_2, L_3 and L_4

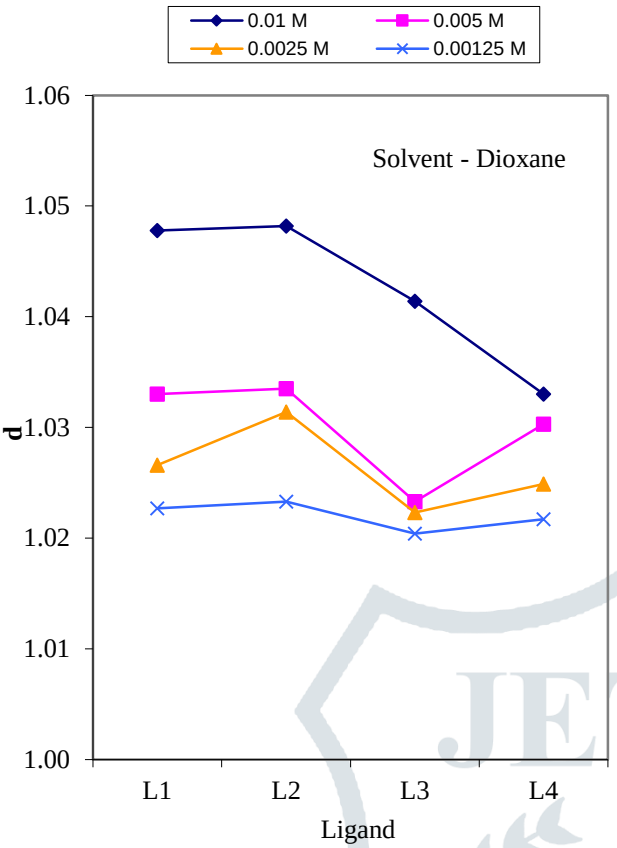


Fig. 2 : Ultrasonic Velocity of L_1, L_2, L_3 and L_4

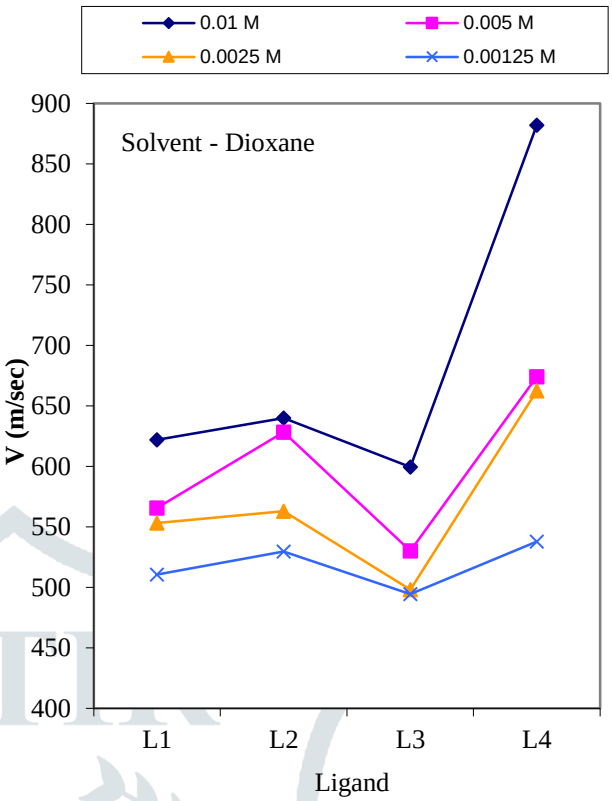


Fig. 3 : Adiabatic compressibility of L1, L2, L3 and L4

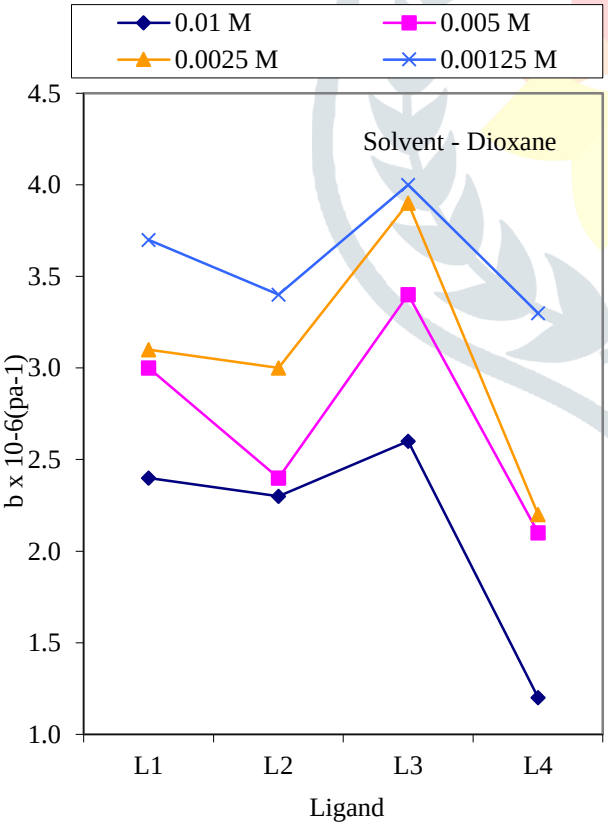


Fig. 4 : Apparent molar compressibility of L1, L2, L3 and L4

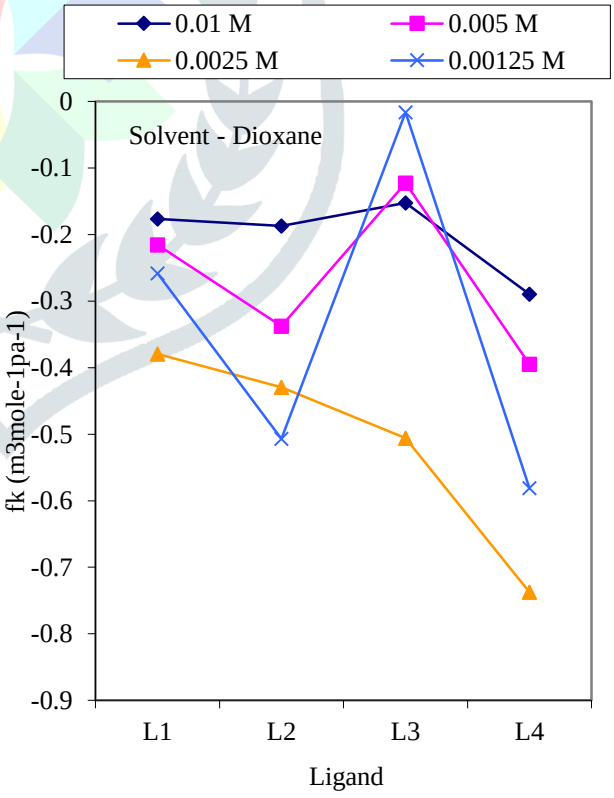
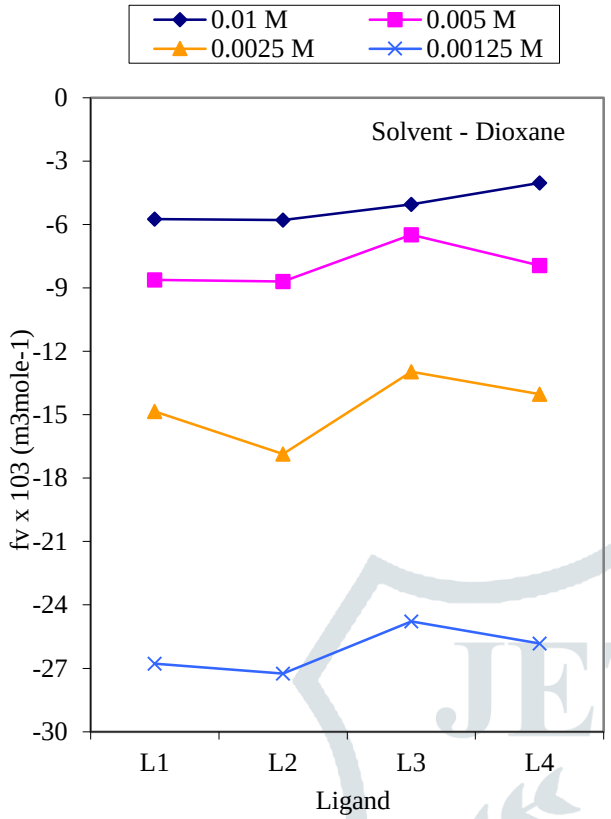


Fig. 5 : Apparent molar volume of L1, L2, L3 and L4



Conclusion

Acoustic parameters such as β, ϕ_v and ϕ_k 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 dioxane at temperature 305.85K 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.

Acknowledgment

The authors are very much thankful to Prof. V. D. Thakare, Head, Department of Chemistry, G.V.I.S.H., Amravati for giving laboratory facilities. They are also thankful to Dr. A.R. Raut, G.V.I.S.H., Amravati and Dr. Naik, Department of Chemical Technology, SGBAU, Amravati for their kind cooperation.

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