Ultrasonic Behaviour and Study of Molecular Interaction of 2-Hydroxy Substituted Quinoxaline in Ethanol Medium

N.A. KALAMBE

Department of Chemistry, P.R. Pote (Patil) College of Engineering & Management, Amravati-444604 (M.S.) India, Corresponding Author: nilimakalambe09@gmail.com

Abstract

Ultrasonic velocity and density measurements of ligand 2-hydroxy substituted quinoxaline were carried out at different percentage of ethanol solvents for investigating solute-solvent, solute-solute interaction 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 (ϕv), apparent molar compressibility (ϕk). The parameters explore solute-solute and solute-solvent interactions in different solvents. In this investigation, the comparative study of effect of solvents and effect of substituents in the solute are studied on molecular interaction of the matter.

Keywords:- Substituted quinoxaline, Acoustic parameters, Interferometry, solute-solvent interaction.

Introduction

Ultrasonic behaviour and study of molecular interaction of substituted 3,5-diaryl isoxazoline in 70% DMF-water mixture at 32°C have been studied by Thorat et al.[1] Ultrasonic interferometric investigations of 3-(Chloroaryl)-5-aryl-1-substituted pyrazoline in dioxane medium[2]. Ultrasonic study of some synthesized pyrazolines at different concentration in 70% of 1,4 dioxane-water mixture[3]. Apparent molar volume of NaCl have been studied in ethanol, methanol, propane-2-ol, dioxane, glycol, glycerol water mixture at 10, 20 and 30% (w/w) within the temperature range 30-40°C and ion solvent interaction has been inferred[4].Ultrasonic and thermodynamical parameters of cinnamaldehyde with o-phenyldiamine in n-Hexane at different temperatute[5] Ultrasonic studies in binary liquid mixtures of trichloro ethylene with three alcohols at 303.15.[6]Variation of acoustical parameters of Dextran in 2(M) Glycine with temperature and concentration.[7] Studies of molecular interaction in the binary mixture of chloroform and methanol by using ultrasonic technique.[8] Ultrasonic studies on molecular interaction in Ternary liquid mixtures at different temperatures.[9] Ultrasonic investigation of intermolecular interactions in binary mixture of isobutyl methyl ketone and acetone.[10] Study of intermolecular interaction in binary mixtures of p-anisaldehyde with bromo-benzene, ethyl-benzene and nitro-benzene at 308.15K[11] Molecular interactions in liquid mixture of 2-hydroxy-5-sulpho benzoic acid in 50% ethanol[12]. Interaction of L-proline in aqueous K_2SO_4, KNO_3 and KCl at temperatures 303.15, 308.15, 318.15 and 323.15 K[13]. Theories of Ultrasonic velocities and their application in the binary liquid mixture of ethyl benzoate with 2-alkoxyethanols at different temperatures.[14].

The use of ultrasound is one of the well recognized approaches for the study of molecular interactions in fluids. The ultrasonic velocity plays and 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 -

(i) 2-(2-Hydroxy-5-chloro)-benzyl-3-phenyl quinoxaline (L_1)

(ii) 2-(2-Hydroxy-5-chloro)-benzyl-3-(4-methoxy phenyl) quinoxaline (L_2)

(iii) 2-(2-Hydroxy-3-bromo-5-chloro)-benzyl-3-phenyl quinoxaline (L_4)

(iv) 2-(2-Hydroxy-3-bromo-5-chloro)-benzyl-3-(4-methoxy phenyl) quinoxaline (L_4)

compounds at different concentration in ethanol solvent separately. The ultrasonic velocity and densities of different concentration in ethanol solvent of L_1, L_2, L_3 and L_4 were determined from those βs, ϕv, ϕk were calculated.

Experimental

All the chemicals were of A.R. grade. Doubly filtered distilled water was used during the study. The solvent ethanol was purified by standard procedure[15]. Densities were measured with the help of bicapillary Pyknometer with difference concentration. Solution of ligand in ethanol solvent prepared separately, that weighed on Mechaniki Zaktady Precynynej 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 ±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 ethanol solvent at temperature 303.85 K.

The adiabatic compressibility of solvent (βo) and (βs) are given by -

$$\beta o = 1/(v_0^2 \cdot do) \quad \text{and} \quad \beta s = 1/(v_s^2 \cdot ds)$$

v_0, do, v_s and ds are ultrasonic velocity and densities of solvent and solution respectively.

Apparent molar volume (ϕv) has been calculated from the relation -

$$\phi v = [1000 (do - ds) / m\ ds\ do] + (M/ds)$$

M = Molecular weight of ligand and m = molarity of the solution.

Apparent molar compressibility (ϕv) was obtained from,

$$\phi k = [1000 (\beta s\ do - \beta o\ ds) / m\ ds\ do] + (\beta s\ M/ds)$$

All these acoustic parameters were computed for all the four ligands at different concentration of ethanol medium.

Results and Discussion

A study of directly β, ϕv and ϕk 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.

Adiabatic compressibility (β)

It is one of the important properties during the study of solute-solvent interactions. The L_2 having higher adiabatic compressibility value than L_3. L_3 have higher β value than L_1 and L_4. The higher values of β for ligands L_2 and L_3 may be due to the presence of chloro and bromo group in the structure.

Table 1 : Acoustic parameters for ligands in Ethanol

Temp. = 305.85 K Ultrasonic Frequency = 1 MHz

Ligand	Conc.	v (m sec^{-1})	d (kg m^{-3})	β x 10^{-6} (pa^{-1})	ϕk (m^{3}mol^{-1}pa^{-1})	ϕv□x 10^3 (m^{3}mol^{-1})
L_1	0.01	347.80	0.9734	8.40	-0.0345	-1.9610
	0.005	412.00	0.9700	6.00	-0.4858	-3.6530
	0.0025	429.08	0.9697	5.60	-1.1122	-7.5501
	0.00125	449.52	0.9598	5.10	-2.4870	-8.0845
L_2	0.01	339.91	0.9773	8.80	-0.0022	-2.3114
	0.005	376.48	0.9749	7.20	-0.2851	-4.5501
	0.0025	399.48	0.9714	6.40	-0.8396	-8.1600
	0.00125	464.72	0.9643	4.80	-2.7350	-11.3864
L_3	0.01	345.69	0.9753	8.50	-0.0266	-2.0610
	0.005	399.50	0.9737	6.40	-0.4966	-5.5239
	0.0025	436.51	0.9710	5.40	-1.1873	-7.9587
	0.00125	454.23	0.9699	4.90	-3.2120	-18.4379
L_4	0.01	382.50	0.9737	7.00	-0.1570	-1.8866
	0.005	428.46	0.9693	5.60	-0.5536	-3.4087
	0.0025	494.34	0.9490	4.30	-1.4680	0.1919
	0.00125	592.00	0.9606	2.90	-4.0146	-8.5615

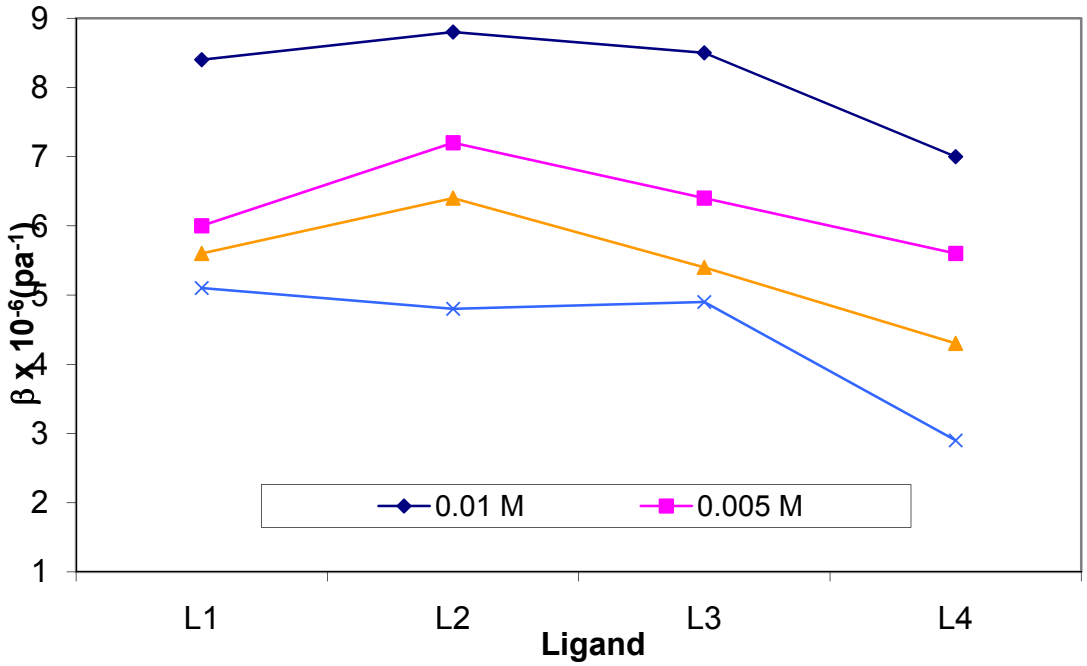

Fig. 1 : Adiabatic compressibility of Ligands L_1, L_2, L_3 and L_4

Apparent molar volume (ϕv)

Apparent molar volume is the thermodynamic property of solutions, which express the solute-solvent interactions. Ligand L4 have higher ϕv value than ligand L3 and L3 have higher ϕv values than L1 and L2. Ethanol have negative value obtained for ligand indicating the compactness of medium and after dissolution of solute due to the closer packing of molecule inside the shell clinging is occurring.

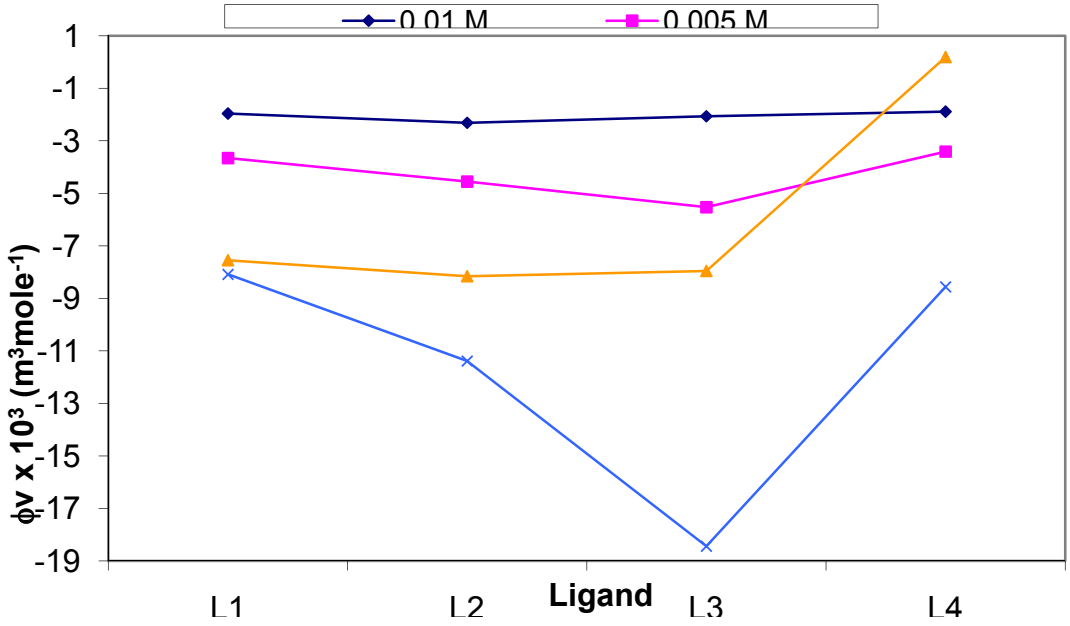

Fig. 2 : Apparent molar volume of Ligands L_1, L_2, L_3 and L_4

Apparent molar compressibility (ϕk)

The structure of solute and the number of atoms present in it will have direct effect on ϕk values. Negative values of ϕk shows that interactions are insensitive to solvent. It could be also explained by postulating the polar -OH group interact with the surrounding organic solvent through dipole-dipole interaction in such a way that the surrounding solvent molecule looses its own compressibility to a certain extent.

Apparent molar compressibility property is fairly sensitive to structural changes especially in highly structured solvent like water, ethanol and is hence expected to throw interesting light[16].

` In ethanol structuredness is already there, the addition of polar solute may break this structuredness of the solvent and form bulk of solute-solvent, as is seen from the lower apparent molar compressibility value.

Conclusion

Acoustic parameters such as β, ϕv and ϕk 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, 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 305.85 K in different concentration.

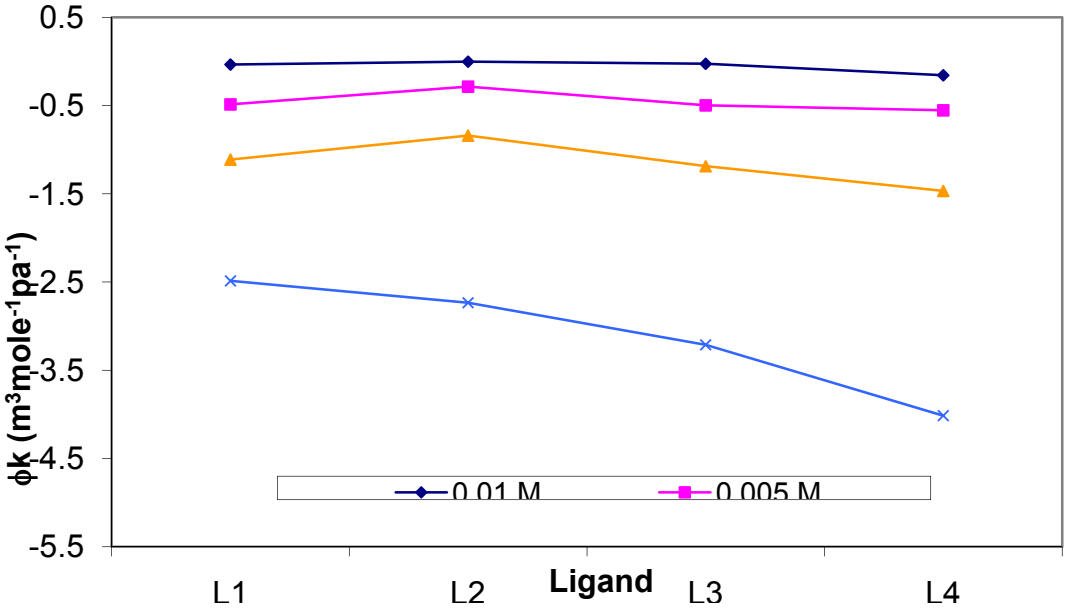

Fig. 3 : Apparent molar compressibility of Ligands L_1, L_2, L_3 and L_4

The above two studied properties of solvent and solutes 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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