SOLUTE-SOLUTE AND SOLUTE-SOLVENT INTERACTIONS OF HYDROXY SUBSTITUTED QUINOXALINE IN CCL_4 SOLVENT AT 297 K

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A B S T R A C T

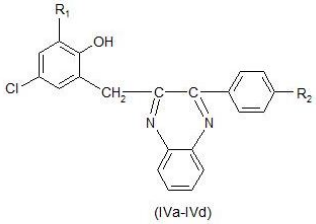
Ultrasonic velocity (v) and density (d) values have been measured in the solvent CCl_4 containing 2-hydroxy substituted quinoxaline using 0.01 M concentration at 297K. From this data, acoustical parameters such as adiabatic compressibility (β_s), apparent molar compressibility (ϕ_k) and relative association (R_A) were determined. 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 quinoxaline, adiabatic compressibility, apparent molar compressibility, relative association

Introduction

The molecular interaction technique play a great role for the detection of molecular association, complex formation, internal pressure. The interferometric method is the most widely used technique for the measuring of sound velocity with high accuracy. Ultrasonic propagation parameters yield valuable information regarding the behaviour of liquid systems, because intermolecular and intermolecular association, dipolar interactions and related structural changes affect the compressibility of the system which in turn produces corresponding variations in the ultrasonic velocity. Solute-solute and solute-solvent interactions of some organic acids in dioxane-water mixtures[1]. Ultrasonic study of isoxazoline at different concentration in 70% of 1,4-dioxane-water mixture[2]. Ultrasonic interferometric investigations of substituted flavones in aqueous ethanol medium at 301 K[3]. Interactions of 1-butyl-3-methyl imidazolium bromide with isopropyl alcohol binary system spectroscopic and volumetric measurements at T (303.15 and 323.15 K)[4]. Intermolecular interaction studies of binary liquid mixtures using time domain reflectometry at 303 K[5]. Theoretical evaluation and experimental study of ultrasonic velocities in binary liquid mixtures of trichloroethylene with three alcohols at 303.15 K[6]. 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 quinoxalines.

2-(2-hydroxy-5-chloro) benzyl-3-(4-methoxy phenyl) quinoxamine (IVa)
2-(2-hydroxy-5-chloro) benzyl-3-phenyl quinoxamine (IVb)
2-(2-hydroxy-3-bromo-5-chloro) benzyl-3-(4-methoxy phenyl) quinoxamine (IVc)
2-(2-hydroxy-3-bromo-5-chloro) benzyl-3-phenyl quinoxamine (IVd)



(IVa-IVd)

Where, R_1 = –H, –Br R_2 = –H, –OCH_3

The above compound of 0.01 M concentration in ethanol studied interferometrically to calculate acoustic parameters velocity (v),

density (d), adiabatic compressibility (β_s), apparent molar compressibility (ϕ_k) and relative association (R_A).

Experimental

All chemicals used to synthesize substituted quinoxaline were of A.R. grade. In this present investigation attempt is made to understand behaviour of 2-hydroxy substituted quinoxaline viz. 2-(2-hydroxy-5-chloro) benzyl-3-(4-methoxy phenyl) quinoxamine (IVa), 2-(2-hydroxy-5-chloro) benzyl-3-phenyl quinoxamine (IVb), 2-(2-hydroxy-3-bromo-5-chloro) benzyl-3-(4-methoxy phenyl) quinoxamine (IVc) and 2-(2-hydroxy-3-bromo-5-chloro) benzyl-3-phenyl quinoxamine (IVd) compounds in CCl4 solvent with respect to v, d, β_s, ϕ_k and R_A.

The solvent CCl_4 was purified by standard procedure[7]. Densities were measured with the help of bicapillary pyknometer, 0.01 M solution of ligand in CCl_4 solvent were prepared separately. Weighing was made on Mechaniki Zaktady Precynyjeij Gdansk balance (± 0.001 g). A special thermostatic arrangement was done for density and ultrasonic viscosity 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 M-815) with accuracy ± 0.03% and frequency 3 MHz was used in the present work. The densities and ultrasonic velocity of liquids in CCl_4 solvent at 297 K.

Results & Discussion

The experimentally determined values of density and ultrasonic velocity for IVa-IVd using CCl_4 solvent at temperature 297 K has been carried out and given in Table 1.

Table 1 - Acoustic parameters for ligands in CCl_4 at 297 K

(Concentration : 0.01 M) (Ultrasonic frequency : 3 MHz)

Ligands	v ($m.sec^{-1}$)	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-6}$ (pa^{-1})	$\phi_k \times 10^{-3}$ ($m^3mol^{-1}pa^{-1}$)	R_A
IVa	639.49	1.7821	4.35777	-47.02304	1.13833
IVb	635.67	1.7815	4.40882	-24.31448	1.14022
IVc	655.16	1.7852	4.15903	-136.56995	1.13115
IVd	646.84	1.7833	4.26217	-89.69908	1.13477

Density (d)

Density measurement have been carried out for different solutions. Density values of CCl_4 medium are higher. This may be due to denser or bulky solvent of CCl_4. Density increases in following order in CCl_4 at 297 K,

IVc > IVd > IVa > IVb

for ligands IVa to IVd. It is 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. Density is the measure of solvent-solvent and ion-solvent interactions.

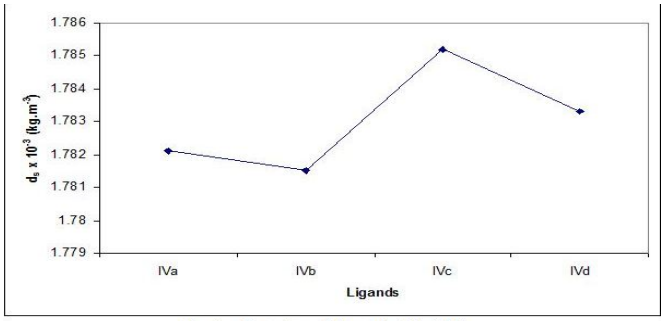


Fig. 1 - Density of ligands IVa-IVd

Velocity (v)

Ultrasonic velocity has been carried out for the different ligands.

In CCl_4 at 297 K, IVc > IVd > IVa > IVb

Ligand IVc have higher velocity due to presence of –Cl, –Br and –OH atoms. The presence of –Br atom which is bigger in size, –I effect of –Cl are acting on the ligand IVc have highest dipole moment. The speed of sound velocity in liquids largely depends on the structure, size, shape and molecular association.

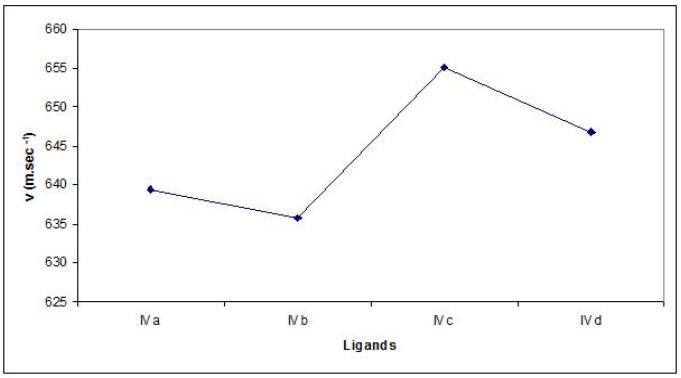


Fig. 2 - Ultrasonic velocity of ligands IVa-IVd

Adiabatic compressibility (β_s)

Adiabatic compressibility is one of the important properties during the study of solute-solvent interactions and represented by β_s.

In CCl_4 at 297 K, IVb > IVa > IVd > IVc

The β_s values in CCl_4 are higher, this may be due to nature of solvent. CCl_4 is a non-polar, low dipole moment and small dielectric constant. The adiabatic compressibility may just explain the simple association or close packing or clinging of molecule.

The positive values of adiabatic compressibility indicates the existence of dispersive forces between molecules of mixtures. It also indicates loosely packed molecules in the mixture.

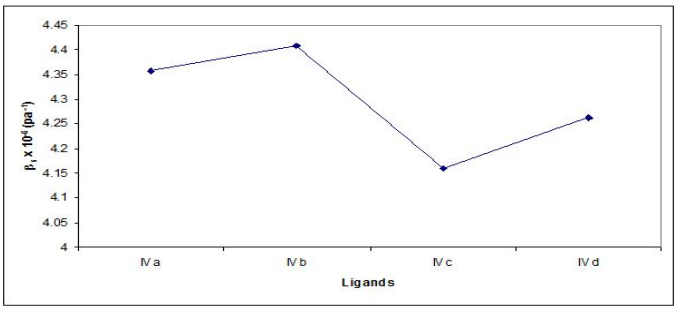


Fig. 3 - Adiabatic compressibility of ligands IVa-IVd

Apparent molar compressibility (ϕ_k)

Apparent molar compressibility (ϕ_k) is another important acoustic parameter, which explains the solute-solvent and solute-solute interactions in solutions. The structure of solute and the number of atoms present in it will have direct effect on ϕ_k values.

It is observed that the ϕ_k values are negative for all ligands in CCl_4. This interprets in terms of loss of compressibility of solute due to strong electrostatic solvation of ions.

In CCl_4 at 297 K, IVb > IVa > IVd > IVc

The negative values of ϕ_k are indicative of ionic and hydrophilic interactions in these systems. ϕ_k provides information regarding solute-solvent interactions. The appreciable negative values of ϕ_k for all of the system reinforce our earlier view about the existence of ion-solvent interactions[8].

Negative values of ϕ_k shows that interaction 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.

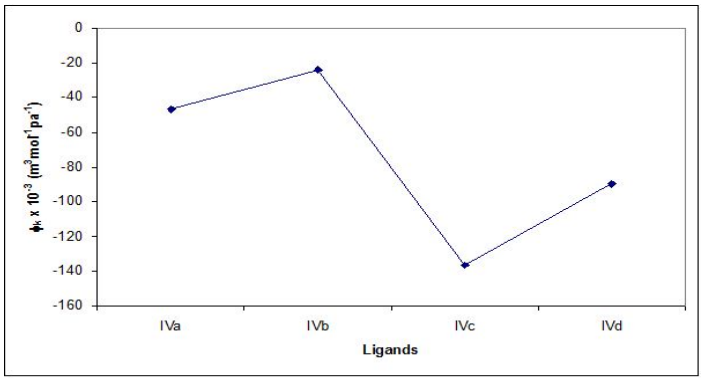


Fig. 4 - Apparent molar compressibility of ligands IVa-IVd

Relative association (R_A)

Relative association is an acoustic property of understanding interaction, which is influenced[9] by two opposing factors; (i) breaking of solvent structure on addition of solute to it, and (ii) solvation of the solutes that are simultaneously present by the free solvent molecules.

In CCl_4 at 297 K

IVb > IVa > IVd > IVc

Relative association affected due to the fact of different withdrawing substituents present in different ligands.

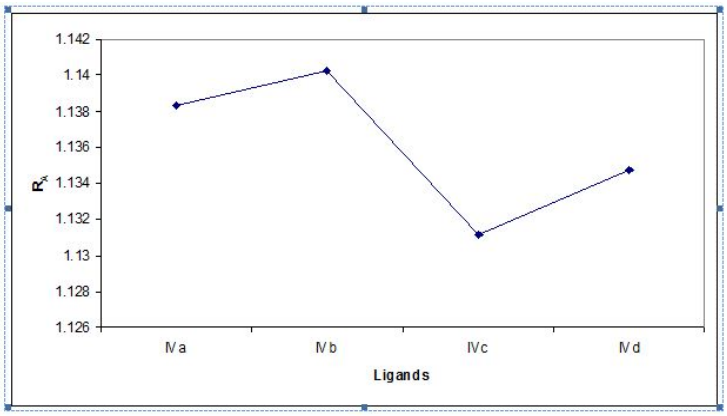


Fig. 5 - Relative association of ligands IVa-IVd

Conclusion

By using ultrasonic interferometric study β_s, ϕ_k, R_A etc. acoustic properties 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 synthesized ligands, which are used as solutes using CCl_4 solvent at 297 K in 0.01 M concentration.

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References

1. Raut, M. P., Raut, A. R. (2016). *IJPRET, 4(9)*, 93-97.
2. Mane, V. D., Mahajan, D. T. (2017). *IJPRET, 6(2)*, 136-144.

3. Sayre, Shubhangi L., Raghuwanshi, Pravin B. (2016). *IJPRET, 4(9),* 77-85.
4. Bennett, Victoria; Ejidibe, P. Ikechukwu; Wankasi, Donbebe; Dikia, D. Ezekiel (2018). *Int. J. Chem. Tech. Res., 11(05),* 209-219.
5. Elangovan, Sampandam; Abbo, Yilak Alemu (2018). *Int. J. Chem. Tech. Res., 11(02),* 196-199.
6. Rao, J. Panduranga; Jyothi, Y., Gopal, K. Nanda; Srinivas G. (2017). *Der Pharma Chemica, 9(4),* 65-72.
7. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., Tatchell, A. R. (2007). *Vogel's Text Book of Practical Organic Chemistry,* 399-400.
8. Dhanlakshmi, A., Jasmine, E., Vasantharani, J. (1999). *Acoustic Soc. Ind., 27,* 327-330.
9. Erying, R., Kincaid, J. F. (1938). *J. Chem. Phys., 6,* 620.