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STUDIES IN THE ACOUSTIC PARAMETERS OF 2–HYDROXY SUBSTITUTED CHALCONE DIBROMIDE IN CCl_4 SOLVENT AT 297 K

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ABSTRACT

Ultrasonic velocity (v) and density (d) values have been measured in the solvent CCl_4 containing 2-hydroxy substituted chalcone dibromide using 0.01 M concentration at 297 K. From this data, acoustical parameters such as adiabatic compressibility (βs), apparent molar volume (ϕ_v), apparent molar compressibility (ϕ_k), intermolecular free length (L_f), relative association (R_A) and specific acoustic impedance (z) have been estimated. These parameters are useful for explaining the molecular association between the components of liquid mixtures. These parameters were studied to solute-solute and solute-solvent interactions in solvent. These parameters provide important and valuable information regarding internal structure, molecular association, complex formation, internal pressure and stability of complexes.

Key words: 2-Hydroxy substituted chalcone dibromide, Acoustic parameters, Solute-solvent interactions, Interferometic study.

INTRODUCTION

The molecular interaction technique play 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. Ultrasonic waves are generally used in studying the properties of matter on the basis of interaction between waves and constituents of the medium through which they pass. Ultrasonic is the branch of acoustic, which consists of waves of high frequencies.

Speed of sound and isentropic compressibilities have been measured for binary

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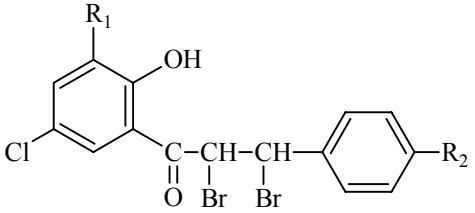
mixtures of 1,2-ethane diol with 1-butanol, 1-hexanol or 1-octanol in the temperature range from 293.15 to 313.15 K[1]. The ultrasonic velocity and density of the binary liquid mixtures of diethyl ether with three non-polar solvents such as carbon tetrachloride, carbon disulphide and benzene at 303.15 K[2]. Investigation in acoustic parameters of substituted thiocarbamido acetophenone[3]. Densities and ultrasonic speed of 2-hydroxy-5-methyl-3-nitro acetophenone in N,N-dimethyl-formamide at different temperature 298.15, 303.15, 308.15 and 313.15 K[4]. Synthesis and acoustical studies of some chalcones of furaldehyde in different solvents at 308.15 K[5].

In view of the analytical, medicinal agricultural, industrial, pharmaceutical significance[6-13], it is of interest to investigate the acoustic parameters such as adiabatic compressibility (βs), apparent molar volume (ϕ_v), apparent molar compressibility (ϕ_k), intermolecular free length (L_f), relative association (R_A) and specific acoustic impedance (z) in CCl_4 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 mixtures[14-19]. But scanty work is found in pure CCl_4 solvent. Also the reviews does not reveal any attempt made on ultrasonic interferometric study of 2-hydroxy substituted chalcone dibromide. We intended to analyze study of these ligands in CCl_4 solvent to investigate protic-aprotic nature, polarity-non-polarity, hydrogen bonding, dielectric constant and density of solvent on solute-solvent, ion-solvent and ion-ion interaction.

EXPERIMENTAL

All chemicals used to synthesize substituted chalcone dibromide were of A.R. grade. In this present investigation attempt is made to understand behaviour of 2-hydroxy substituted chalcone dibromide viz. 2'-hydroxy-5'-chloro-4-methoxy chalcone dibromide (IIIa), 2'-hydroxy-5'-chloro chalcone dibromide (IIIb), 2'-hydroxy-3'-bromo-5'-chloro-4-methoxy chalcone dibromide (IIIc) and 2'-hydroxy-3'-bromo-5'-chloro chalcone dibromide **(IIId)** compounds in CCl_4 solvent with respect to v, d, β_s, ϕ_v, ϕ_k, L_f, R_A and z.



(IIIa-d)

Where, R_1 = –H, –Br R_2 = –H, $–OCH_3$

The solvent CCl_4 were purified by standard procedure[20]. Densities were measured with the help of bicapillary pyknometer. 0.01 M solution of liquid 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 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 M-81S) 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 AND DISCUSSION

In the present investigation measurement of densities and ultrasonic velocities of **IIIa** to **IIId** in CCl_4 has been carried out and given in Table 1.

Table 1: Acoustic parameters for ligands in CCl_4 at 297K (Concentration: 0.01 M; Frequency: 3 MHz)

Ligands	V (m. sec^{-1})	ds x 10^3 (Kg.m^{-3})	βs x 10^{-6} (pa^{-1})	ϕ_k x 10^{-3} ($m^3mol^{-1}pa^{-1}$)	ϕ_v x 10^{-3} (m^3mol^{-1})	L_f (m^{-1})	R_A	Z (Kg $m^{-2}sec^{-1}$)
IIIa	651.53	1.7841	4.20291	-116.26681	-62.3583	1.30386	1.13254	1162.395
IIIb	642.28	1.7828	4.32169	-63.34275	-61.968	1.32215	1.13713	1145.057
IIIc	664.46	1.7869	4.04727	-186.9568	-63.19282	1.27949	1.12692	1187.324
IIId	659.34	1.7861	4.10853	-159.45869	-62.9583	1.28914	1.12932	1177.647

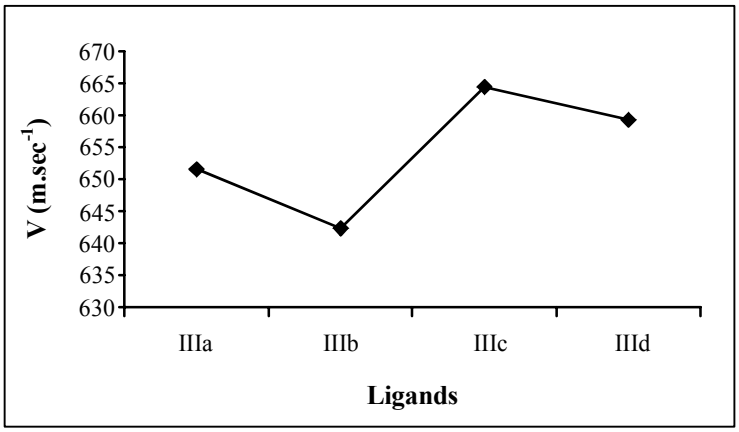


Fig. 1: Ultrasonic velocity of ligands IIIa-IIId

Density (d)

Density measurements 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,

IIIc > IIId > IIIa > IIIb

for ligands **IIIa** to **IIId**. It is due to presence of $\tilde{}$OH, $\tilde{}$Cl, $\tilde{}$Br groups, these group show -I effect and +R effect of which latter predominates +R effect increases the electron density.

Velocity (v)

Ultrasonic velocity has been carried out for different the solutions.

In CCl_4 at 297 K,

IIIc > IIId > IIIa > IIIb

Ligand **IIIc** 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 $\tilde{}$Cl are acting on the ligand IIIc have highest dipole moment.

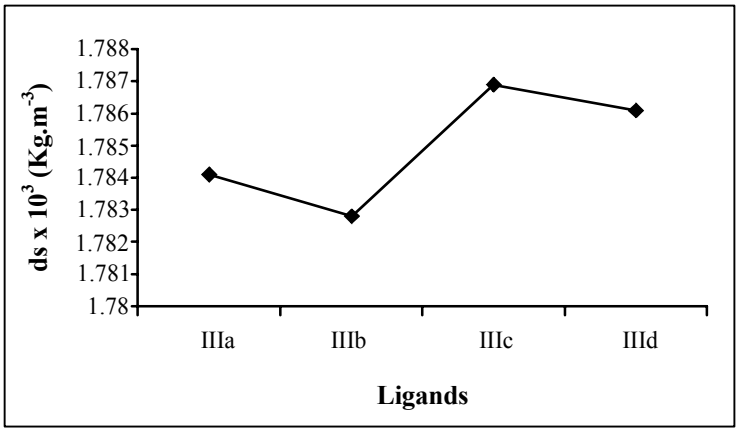


Fig. 2: Density of ligands IIIa-IIId

Adiabatic compressibility (βs)

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

In CCl_4 at 297 K,

IIIb > IIIa > IIId > IIIc

The β 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 molecules.

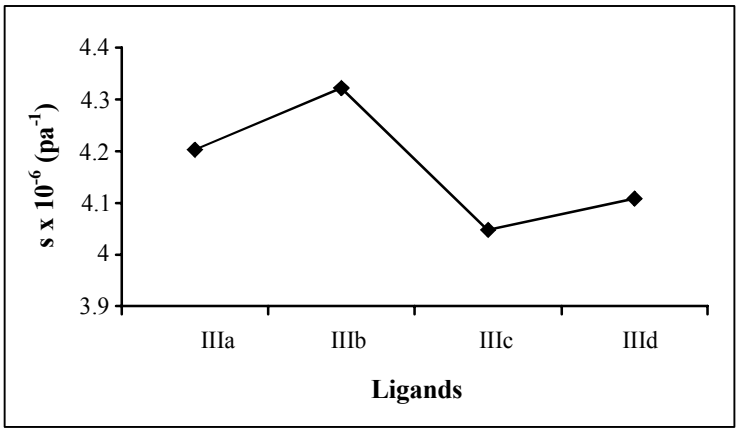


Fig. 3: Adiabatic compressibility of ligands IIIa-IIId

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,

IIIb > IIIa > IIId > IIIc

The negative values of ϕ_k are indicative of ionic and hydro-phillic 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[21].

Negative value 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.

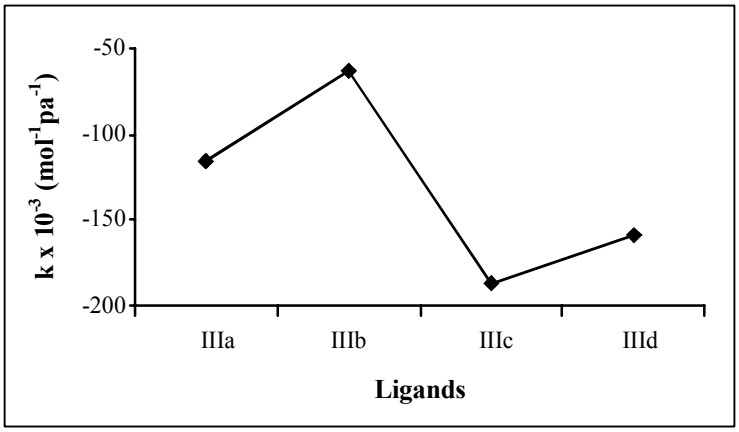


Fig. 4: Apparent molar compressibility of ligands IIIa-IIId

Apparent molar volume (ϕ_v)

Apparent molar volume is the thermodynamic property of solutions, which express the solute-solvent interactions, and it is obtained from the density and molarity of solution and the molecular weight of the solute.

In CCl_4 at 297 K,

IIIb > IIIa > IIId > IIIc

It is observed that ϕ_v values are negative for all ligands in CCl_4. Negative value obtained for ligand indicating the compactness of medium and after dissolution of solute due to the closer packing of molecules inside the shell more clinging is occurring. The negative values of ϕ_v for the system indicate the existence of smaller solute-solute interactions[22].

Intermolecular free length (L_f)

It is one of the important acoustic properties to study the intermolecular interactions.

In CCl_4 at 297 K,

IIIb > IIIa > IIId > IIIc

The decrease in intermolecular free length values indicating that there is a significant interaction between solute and solvent molecules[23] suggesting a structure promoting behaviour on the addition of solute.

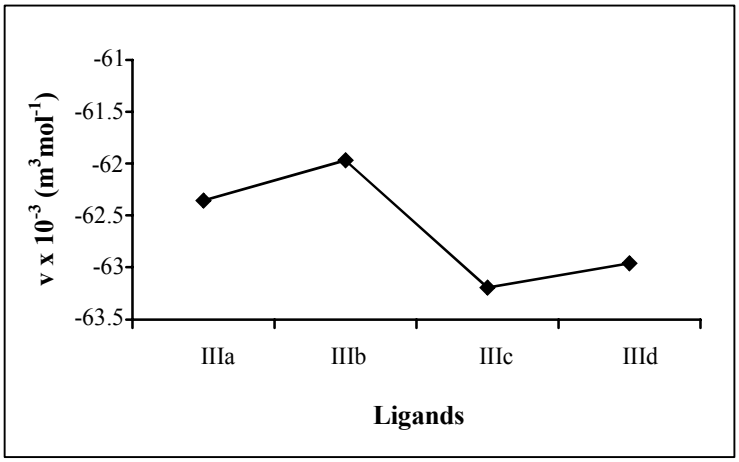


Fig. 5: Apparent molar volume of ligands IIIa-IIId

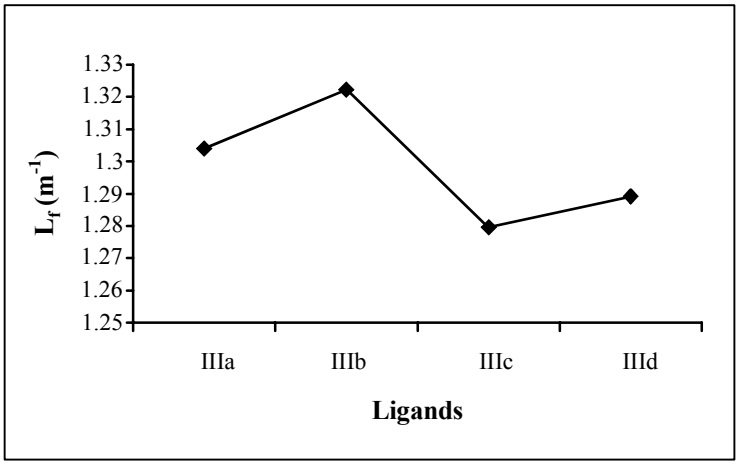


Fig. 6: Intermolecular free length of ligands IIIa-IIId

The intermolecular free length depends upon the intermolecular attractive and repulsive forces. L_f is a predominating factor in determining the variation of ultrasonic velocity of solution. There is a significant interaction between solute and solvent molecules due to which its structural arrangement is also affected[24].

Relative association (R_A)

Relative association is an acoustic property of understanding interaction, which is influenced[25] 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,

IIIb > IIIa > IIId > IIIc

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

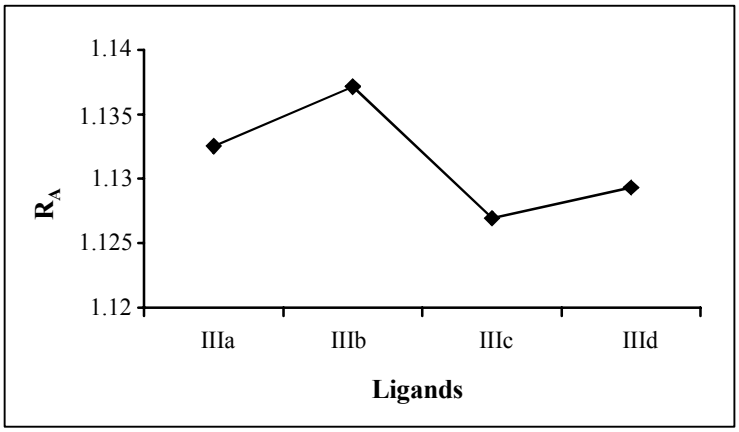


Fig. 7: Relative association of ligands IIIa-IIId

Specific acoustic impedance (z)

Specific acoustic impedance is the complex ratio of the effective sound pressure at a point to the effective particle velocity at that point[26].

In CCl_4 at 297 K,

IIIc > IIId > IIIa > IIIb

The values of z are continuously decreasing on changing the structure of ligand. The specific acoustic impedance depends upon the various structure of the liquid and the molecular packing in the medium.

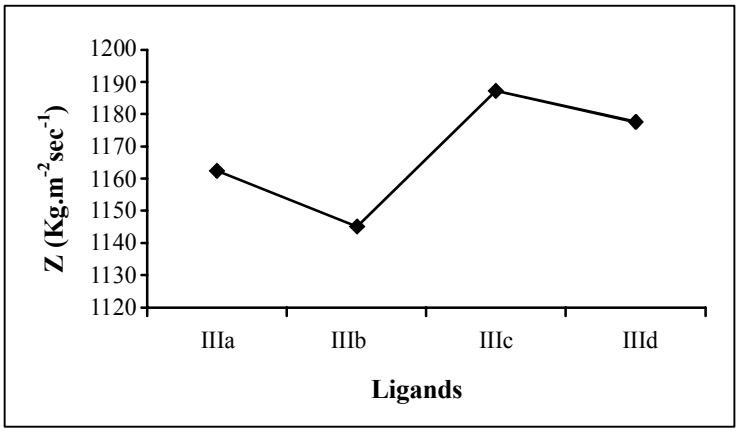


Fig. 8: Specific acoustic impedance of ligands IIIa-IIId

CONCLUSION

By using ultrasonic interferometric study β, ϕ_v, ϕ_k, L_f, R_A, z 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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