

Acoustic parameters of some 1-3 thiazine in binary mixture of 70% dioxane + water

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Abstract - Thiazine is six membered heterocyclic ring containing Nitrogen and Sulphur placed at 1, 3 position. In present investigation complex formation between thiazine and solvent are studied by evaluating certain acoustic parameter. The Complex formation in binary liquid mixtures of 1-4 dioxane and water with 4-(2-hydroxy phenyl)-5 benzoyl-6-(4-methoxyphenyl)-2-imino-6H-2,3-dihydro-1,3 thiazine L2, 4-(2-hydroxy phenyl)-5 benzoyl-6-(2-furyl)-2-imino-6H-2,3-dihydro-1,3 thiazine L3, 4-(2-hydroxy -5-methyl phenyl)-5 benzoyl-6-(4-methoxyphenyl)-2-imino-6H-2,3-dihydro-1,3 thiazine L5 has been studied by measuring ultrasonic velocity at 2 MHz, by using in the concentration range of 0.01 M at 32 °C the parameters under investigation are ultrasonic velocity (u), adiabatic compressibility (β_s), intermolecular free length, (L_f) Apparent molal volume (Φ_v), Apparent molal Compressibility (Φ_k), specific acoustic impedance (Z) and Relative association (RA) These parameters have been utilized to study the solute-solute interactions in these systems. The ultrasonic velocity shows a decrease in value with respect to concentration and adiabatic compressibility show corresponding increase in value with respect to concentration for these ligands. The results indicate the occurrence of complex formation between unlike molecules through intermolecular hydrogen bonding between oxygen atom of dioxane molecule and hydrogen atom of ligands. The variation of these parameters with percentage indicates the possibility of the complex formation in these systems.

Index Terms - Acoustical impedance, Dioxane-water mixtures, thiazine.

INTRODUCTION - Ultrasonic is the branch of acoustic, which consists of waves of high frequencies. Ultrasonic study has wide range of application in agriculture, material science, medicine, biology, industry, oceanography, sonochemistry research as it have a non-destructive nature¹. This technique is used for the study of molecular interaction in liquids.²⁻⁵ It is also useful to study the ion-solvent interactions in aqueous and non aqueous solutions⁶. Recent developments have made it possible to use ultrasonic energy in medicine, engineering, agriculture and other industrial applications⁷⁻⁸.

In solution of ionic solute the attraction between the solute and solvent is essentially of ion-dipole interaction depends mainly on ion size and polarity of the solvent⁹. The measurements of ultrasonic waves are useful in study of molecular interactions in liquids which provides valuable information regarding internal structure, complex formation, internal pressure and molecular association¹⁰. The dissolution of electrolyte in a solvent causes a volume contraction due to interaction between ions and solvent molecules and this may influence other acoustical properties of solution. In recent years, the studies of acoustical properties of aqueous mixed electrolytic solutions¹¹ have been found to be useful in understanding the specific ion-ion and ion-solvent interaction in solutions. The strength of ion-dipole attraction is directly proportional to the size of the ion, charge and the magnitude of the dipole, but inversely proportional to the distance between the ion and the dipolar molecule. The accurate measurement of density, viscosity, ultrasonic velocity and hence the derived parameters such as adiabatic compressibility, apparent molal compressibility and apparent molal volume will give significant information regarding the state of affairs in a solution¹².

I. RESEARCH METHODOLOGY

The 1,3 substituted thiazine are synthesized by amination of chalcone with substituted amines, this chalcone are synthesized by using general Claisen Schmidt method. For evaluating the acoustic properties the very pure and analytical grade solvent (1-4 Dioxane) and extra pure double distilled water is used. The densities of pure solvent and solutions are determined by using specific gravity bottle. The ultrasonic velocity measurements were made using a crystal controlled variable path ultrasonic interferometer (Mittal Enterprise, Model F-05) of 2MHz with accuracy of (\pm) 0.03 %

The ligands used for study are

1] 4-(2-hydroxy phenyl)-5 benzoyl-6-(4-methoxyphenyl)-2-imino-6H-2,3-dihydro-1,3 thiazine L2

2] 4-(2-hydroxy phenyl)-5 benzoyl-6-(2-furyl)-2-imino-6H-2,3-dihydro-1,3 thiazine L3

3] 4-(2-hydroxy -5-methyl phenyl)-5 benzoyl-6-(4-methoxyphenyl)-2-imino-6H-2,3-dihydro-1,3 thiazine L5

II. THEORY AND CALCULATION

Adiabatic compressibility (β), Apparent molal volume (Φ_v), Apparent molal compressibility (Φ_k), Intermolecular free length (L_f), Specific acoustic impedance (Z) and Relative association (R) were calculated by using following equations

$$\beta_s = 100 / (U_s^2 ds) \quad \dots\dots\dots 1$$

$$\beta_o = 100 / U_o^{2*} d_o \quad \dots\dots\dots 2$$

$$\phi_v = (M/ds) + [(d_o - ds)10^3] / m ds d_o \quad \dots\dots\dots 3$$

$$\phi_k(s) = [1000 (\beta_s d_o - \beta_o ds) / m ds d_o] + (\beta_s M / ds) \quad \dots\dots 4$$

$$L_f = K \times \sqrt{\beta_s} \quad \dots\dots\dots 5$$

$$Z = U_s ds \quad \dots\dots\dots 6$$

where,

d_o = Density of pure solvent,

m = Molality, M = Molecular weight of solute,

β_o = Adiabatic compressibility of pure solvent

β_s = Adiabatic compressibility of solution

K = Jackson's constant

U_s = Ultrasonic velocity in the solution in m/s.

β_s is in bar^{-1} and $\phi_k(s)$ is in $\text{cm}^3 \text{mol}^{-1} \text{bar}^{-1}$

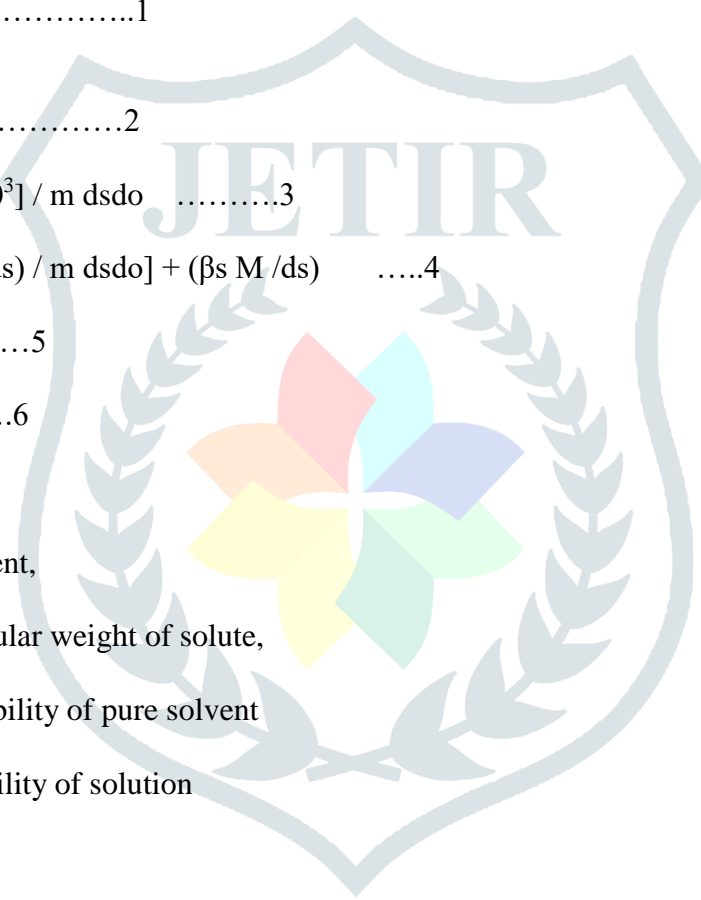


Table - 1 Acoustic parameters of ligand L2 in 70% dioxane-water system

% DIOXANE	Mole fraction of DIOXANE	Ultrasonic Velocity (u) (m/sec) ×10 ³	Density (ds) (g/m ²) ×10 ⁶	Adiabatic compressibility β _s (bar ⁻¹) ×10 ⁻⁷	Intermolecular free length L (A ₀) ×10 ⁻⁹	Apparent molal volume Φ (m ³ /mole) ×10 ⁻³	Apparent molal Compressibility (Φ) (m ³ mol ⁻¹ k(s) bar ⁻¹) ×10 ⁻⁴	Relative association (R)	Specific acoustic impedance Z _s (kg m ⁻² s ⁻¹) ×10 ⁶
100	1	3332	1.0556	0.853244	0.601	7075.684	1.05	0.5240	3517.399
90	0.6563	2684.4	0.9545	1.4538	0.7.84	14046.09	2.03	0.8369	2562.399
80	0.4584	2074	0.9028	2.57487	1.04	14889.72	3.59	1.1451	1872.561
70	0.3305	1906	0.8588	3.20516	1.16	18202.23	4.50	1.2524	1636.922
60	0.2409	1712.8	0.8211	4.150907	1.32	23345.91	5.94	1.3832	1406.509

Table - 2 Acoustic parameters of ligand L3 in 70% dioxane-water system

% DIOXANE	Mole fraction of DIOXANE	Ultrasonic Velocity (u) (m/sec) ×10 ³	Density (ds) (g/m ²) ×10 ⁶	Adiabatic compressibility β _s (bar ⁻¹) ×10 ⁻⁷	Intermolecular free length L (A ₀) ×10 ⁻⁹	Apparent molal volume Φ (m ³ /mole) ×10 ⁻³	Apparent molal Compressibility (Φ) (m ³ mol ⁻¹ k(s) bar ⁻¹) ×10 ⁻⁴	Relative association (R)	Specific acoustic impedance Z _s (kg m ⁻² s ⁻¹) ×10 ⁶
100	1	3332	1.0556	0.853244	0.601	7075.684	1.05	0.5240	3517.399
90	0.6563	2684.4	0.9545	1.4538	0.7.84	14046.09	2.03	0.8369	2562.399
80	0.4584	2074	0.9028	2.57487	1.04	14889.72	3.59	1.1451	1872.561
70	0.3305	1906	0.8588	3.20516	1.16	18202.23	4.50	1.2524	1636.922

60	0.2409	1712.8	0.8211	4.150907	1.32	23345.91	5.94	1.3832	1406.509
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Table - 3 Acoustic parameters of ligand L5 in 70% dioxane-water system

% DIOXANE	Mole fraction of DIOXANE	Ultrasonic Velocity (u) (m/sec) ×103	Density (ds) (g/m ²) ×106	Adiabatic compressibility βs (bar ⁻¹) ×10 ⁻⁷	Intermolecular free length L (A0) ×10 ⁻⁹	Apparent molal volume Φ (m ³ /mol) ×10 ⁻³	Apparent molal Compressibility (Φ) (m ³ mol ⁻¹ k(s) bar ⁻¹) ×10 ⁻⁴	Relative association (R)	Specific acoustic impedance Zs (kg m ⁻² s ⁻¹) ×106
100	1	3332	1.0556	0.853244	0.601	7075.684	1.05	0.5240	3517.399
90	0.6563	2684.4	0.9545	1.4538	0.7.84	14046.09	2.03	0.8369	2562.399
80	0.4584	2074	0.9028	2.57487	1.04	14889.72	3.59	1.1451	1872.561
70	0.3305	1906	0.8588	3.20516	1.16	18202.23	4.50	1.2524	1636.922
60	0.2409	1712.8	0.8211	4.150907	1.32	23345.91	5.94	1.3832	1406.509

III. RESULTS AND DISCUSSION

In the present investigation different acoustic parameters such as adiabatic compressibility (β), apparent molal volume (Φ_v), apparent molal compressibility (Φ_k), acoustic impedance (Z), relative association (RA) and intermolecular free length (L_f) of the solutions in 0.01M concentrations of solute are determined at 303k and presented in table 1(A)& 1(B).

The ultrasonic velocity of both the ligand is going to decrease with decrease in percentage of dioxane this indicates decrease the cohesion which is caused due to hydrogen bonding. The value of adiabatic compressibility increase (β_s) with decrease in percentage of solution may be due to departure of solvent molecules around ions supporting weak ion-solvent interactions. increases linearly in both the compound which represents the interaction of solute and solvent is weak. Value of adiabatic compressibility β_s is more for FB ligand than CFB show that FB have strong solute solvent interaction. The value of apparent molal volume (Φ_v) is high in case of more polar substituent than less polar substituents. The apparent molal volume Φ_v values increases with decrease in concentration of chalconesimines in binary mixtures this represents strong solute-solute and solute solvent interactions. Relative association RA increases linearly with decrease in percentage. It is influenced by breaking of bond in ions. Decrease in RA with decrease in concentration suggests that breaking up of dioxane aggregation predominates the solvation of ions. The value of relative association increases with decrease in concentration in all systems. It is found that there is weak interaction between solute and solvent. Relative association is more in case of bulky and more polar substituents

The value of apparent molal compressibility (Φ_k) increases with decrease in percentage of all systems, Showing weak electrostatic attractive force in the vicinity of ions causing electrostatic solvation of ions. Compressibility is more in case of bulky substituents The values of intermolecular free length (L_f) indicates that with increase in concentration there is increase in ion-solvent interactions. The intermolecular free

length increases due to greater force of interaction between solute and solvent by forming hydrogen bonding and less interaction between two solute molecules.

IV. CONCLUSION

From the experimental data, density and compressibility data have been determined for halosubstituted chalconeimine in binary liquid (dioxane+water at 32^oC) the results have been used to study the ion-solvent interaction exists in the mixture. From the magnitude of ϕk and β -coefficient values it can be concluded that the existence of ion-solvent interaction is in the order: NiSO₄ > MnSO₄ > CoSO₄. The transfer volume $\Delta\phi$ suggests the predominance of hydrophilic-hydrophobic interactions over ionohydrophilic interactions. From the co-sphere overlap model it can be concluded that ion-solvent interactions are dominating over the solute-co-solute interactions.

V. ACKNOWLEDGMENT

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VI. REFERENCES

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