Non-Destructive Evaluation of 2-Mercapto Substituted Pyrimidine Derivatives in Different Concentration and Different Percentages in Dioxane-Water Mixture

Pravin S. Bodke, Shradha S. Binani, Ravi V. Joat

***Abstract*—**Science and technology of ultrasonic is widely used in recent years for industrial and medicinal application. The acoustical properties of 2-mercapto substituted pyrimidines viz.,2- Mercapto-4-(2',4' –dichloro phenyl) – 6-(2' – hydroxyl -4' –methyl-5' – chlorophenyl) pyrimidine and 2 –Mercapto – 4-(4' –chloro phenyl) – 6-(2' – hydroxyl -4' –methyl-5' –chlorophenyl) pyrimidine have been investigated from the ultrasonic velocity and density measurements at different concentration and different % in dioxane-water mixture at 305K. The adiabatic compressibility (β_s), acoustic impedance (Z), intermolecular free length (L_f), apparent molar volume(ϕ_v) and relative association (R_A) values have been calculated from the experimental data of velocity and density measurement at concentration range of 0.01- 0.000625 mol/lit and 70%,75% and 80% dioxane water mixture. These above parameters are used to discuss the structural and molecular interactions.

***Keywords*—**Acoustical parameters, Density, Dioxane-water mixture, Ultrasonic velocity.

I. Introduction

ULTRASONICwave's means sound waves hearing above range of normal ear. The study of intermolecular interaction plays an important role in the development of molecular sciences. The nature and relative strength of the molecular interaction between the components of the liquid mixtures have been studied by the ultrasonic method. A large number of studies have been made on the molecular interaction in liquid mixtures by various physical methods like ultra-violet, infrared, nuclear magnetic resonance, dielectric constant, Raman effect and ultrasonic method [1]-[4]. For interpreting solute-solvent, ion-solvent interaction in aqueous and non-aqueous medium was helpful from Ultrasonic velocity measurements in recent year [5], [6] .Ultrasonic waves used to detect a wide variety of anomalous condition such as pregnancy, tumors and a study various phenomena such as heart valve action. This ultrasonic wave is more sensitive than X-rays. Due to this ultrasonic technique used in the treatment of certain cancer as well as arthritis and related diseases [7]. The studies of the determination of densities, viscosities, refractive indices of organic liquid mixture are reported by many workers [8] Ramteke et al. reported acoustical properties of chloro-substituted pyrazoles in different concentration and different % in dioxane–water mixture [9]. Substituted pyrimidines and their derivatives have received much attention towards their application in agro chemical industries and medicinal values. The chloro substituted pyrimidines act as an antimicrobial drugs [10] and in view of applications in various fields. The work follow systematic studies of chloro substituted pyrimidines in different concentration and different percentage in dioxane-water and measure the ultrasonic velocities and densities and from those values, various acoustic properties had been evaluated.

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II. Materials and Methods

All chemicals were used of analytical grade was purified by vogel's standard method. The distilled dioxane was used for preparation of different concentration and different percentages of chloro substituted pyrimidine solution. Acetone was used for washing purpose. The acoustical properties require the measurement of ultrasonic velocity and densities. The densities of pure solvent and their solution were measured by using densitometer. The ultrasonic velocities were measured by using. In the present work, different properties such as adiabatic compressibility (β_s), apparent molal volume (ϕ_v), intermolecular free length (L_f), apparent molal compressibility (ϕ_k), acoustic impedance (Z), relative association (R_A) have been evaluated from following equations.

The adiabatic compressibility (β_s) was calculated from Newton-Laplace.

$$\beta_s = 1/U_s \text{ x } d_s \text{ [for solution]} \quad (1)$$

$$\beta_o = 1/U_o \text{ x } d_o \text{ [for solvent]} \quad (1a)$$

where d_s, d_o and U_s, U_o are the densities of pure solvent, solution and ultrasonic velocities of pure solvent and solutions, respectively.

The apparent molal compressibility (ϕ_k) has been calculated by using the relation.

$$\phi_k = 1000 (\beta_s \text{ x } d_o - \beta_o \text{ x} d_s) / m \text{ x } d_s \text{ x } d_o + \beta_s \text{ x } M / d_s \quad (2)$$

The apparent molal volume (ϕ_v) has been evaluated by using the relation.

$$\Phi_v = M / d_s+(d_o-d_s)x10^3 / m \times d_s \times d_o \quad (3)$$

where, M is the molecular weight of solute and ' m' is the molality of the solute.

The inter molecular free length (L_f) is calculated by using the standard expression

$$(L_f)= K \times \sqrt{\beta_s} \quad (4)$$

where K is temperature dependent constant known as Jacobson's constant.

The relative association (R_A) was calculated by the following equation

$$R_A= [d_s/d_o] [U_o /U_s]^{1/3} \quad (5)$$

The acoustic impedance (Z) is obtained by the following relation

$$Z= d_s \times U_s \quad (6)$$

III. Result and Discussion

The experimental values of density and ultrasonic velocity at different concentration of ligand (L_1& L_2) and different percentage in dioxane –water mixtures at 305K are given in Tables I and II.

TABLE I
VALUES OF DENSITY AND ULTRASONIC VELOCITY AT DIFFERENT CONCENTRATION OF LIGAND L_1AND L_2 AT 305K

Concentration (mole/lit.)	√c	Density (g/cm^3)		Ultra Sonic Velocity (m/sec)	
		L_1	L_2	L_1	L_2
0.01	0.100	1.0175	1.0284	1428.6	1463.0
0.005	0.070	1.0163	1.0163	1436.4	1472.0
0.0025	0.050	1.0028	1.0134	1439.3	1474.0
0.00125	0.035	1.0014	1.0089	1442.7	1484.1
0.000625	0.025	0.9625	0.9831	1451.9	1492.2

TABLE II
VALUES OF DENSITY AND ULTRASONIC VELOCITY AT DIFFERENT PERCENTAGES IN DIOXONE- WATER MIXTURE IN 305K

% of Dioxane	Density (g/cm^3)		Ultrasonic Velocity (m/sec)	
	L_1	L_2	L_1	L_2
70%	1.0389	1.0262	1448.9	1494.0
75%	1.0231	1.0168	1436.2	1463.0
80%	1.0214	1.0037	1428.4	1448.0

In Tables I and II, L_1 denotes 2-Mercapto – 4-(2', 4' –dichloro phenyl)–6-(2'– hydroxyl -4'–methyl-5'–chlorophenyl) pyrimidine values and L_2 denotes 2 – Mercapto – 4-(4' –chloro phenyl) – 6-(2'–hydroxyl -4' –methyl-5' –chlorophenyl) pyrimidine values which have been used to determine the acoustical properties of 2-mercapto substituted pyrimidines at different concentration and different percentage which are given in Tables III, IV, V and VI respectively.

TABLE III
ACOUSTIC PROPERTIES OF LIGAND (L_1) OF DIFFERENT CONCENTRATION IN DIOXANE-WATER MIXTURE AT 305K

Different conc, (mol.lit^{-1})	β_s X 10^{-7} (bar^{-1})	Φ_v x 10^2 (cm^3.mol^{-1})	Φ_k x 10^{-4} (cm^3.mol^{-1}.bar^{-1})	L_f x 1C (A°)	R_A	Z x 10^2 cm.sec^{-1}. g.cm^{-3}
0.01	4.5446	5.0521	2.5395	4.4345	1.0197	1440.41
0.005	4.3518	5.0445	2.4503	4.3435	1.0075	1556.01
0.0025	4.2814	5.0405	2.3085	4.3098	1.0052	1573.26
0.00125	4.1714	5.0257	2.2013	4.2051	1.0048	1582.73
0.000625	4.0233	5.0145	2.1723	4.1518	1.0036	1598.96

TABLEIV
ACOUSTIC PROPERTIES OF LIGAND (L_2) OF DIFFERENT CONCENTRATION IN DIOXANE-WATER MIXTURE AT 305K

Different conc, (mol.lit^{-1})	β_s X 10^{-7} (bar^{-1})	Φ_v x 10^2 (cm^3.mol^{-1})	Φ_k x 10^{-4} (cm^3.mol^{-1}.bar^{-1})	L_f x 1C (A°)	R_A	Z x 10^2 cm.sec^{-1}. g.cm^{-3}
0.01	4.5295	3.9474	1.7286	4.3756	1.0337	1516.25
0.005	4.5822	3.9893	1.8045	4.3957	1.0192	1493.24
0.0025	4.7654	4.1581	1.9248	4.4042	0.9237	1449.70
0.00125	4.7878	4.2896	1.9403	4.4592	0.8968	1432.02
0.000625	4.8584	4.3525	2.1046	4.5331	0.8238	1380.75

TABLE V
ACOUSTIC PROPERTIES OF LIGAND (L_1) OF DIFFERENT PERCENTAGES IN DIOXANE-WATER MIXTURE AT 305K

% of Dioxane	β_s X 10^{-7} (bar^{-1})	Φ_v x 10^2 (cm^3.mol^{-1})	Φ_k x 10^{-4} (cm^3.mol^{-1}.bar^{-1})	L_f x 1C (A°)	R_A	Z x 10^2 cm.sec^{-1}. g.cm^{-3}
70%	4.518	5.0421	2.3622	4.3486	1.0175	1483.85
80%	4.696	5.0634	2.3976	4.3637	1.0164	1471.03
90%	4.787	5.0785	2.4226	4.4012	1.0043	1462.48

TABLE VI
ACOUSTIC PROPERTIES OF LIGAND (L_2) OF DIFFERENT PERCENTAGES IN DIOXANE-WATER MIXTURE AT 305K

% of Dioxane	β_s X 10^{-7} (bar^{-1})	Φ_v x 10^2 ($cm^3.mol^{-1}$)	Φ_k x 10^{-4} ($cm^3.mol^{-1}.bar^{-1}$)	L_f x 1C (A°)	R_A	Z x 10^2 $cm.sec^{-1}. g.cm^{-3}$
70%	4.6195	3.8774	1.8986	4.1756	1.0137	1608.25
80%	4.7375	3.9204	1.9219	4.2312	1.0537	1597.45
90%	4.9765	4.1051	1.9854	4.3414	1.0747	1547.16

The various acoustical properties like adiabatic compressibility (β_s), apparent molal volume (Φ_v), intermolecular free length (L_f), apparent molal compressibility (Φ_k), acoustic impedance (Z), relative association (R_A) which are calculated using above equation and which are represented in Tables III-IV.

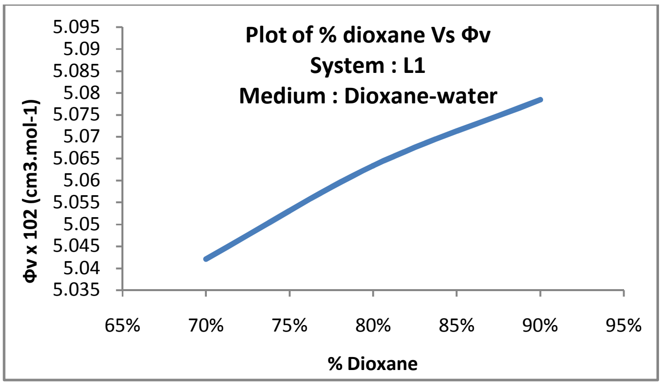

Fig. 1 % dioxane Vs apparent molal volume (L_1)

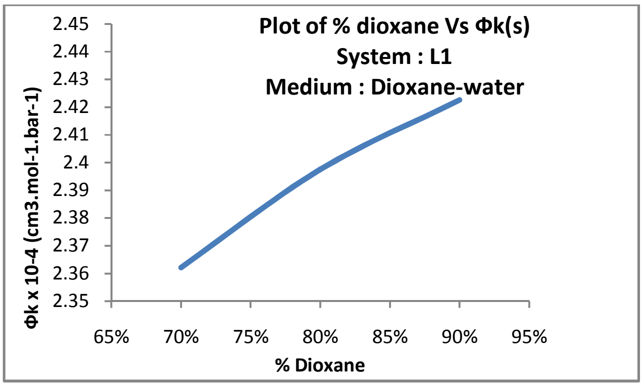

Fig. 2 % dioxane Vs apparent molal compressibility (L_1)

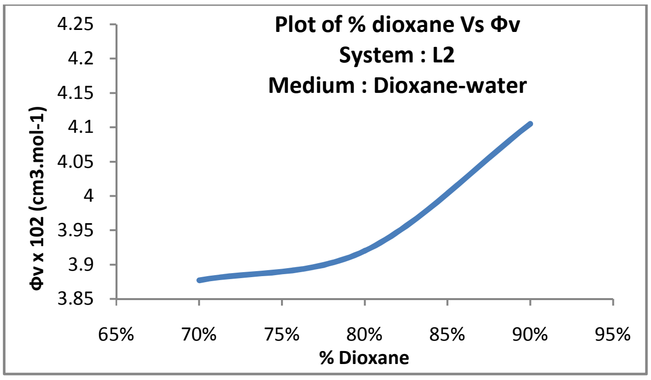

Fig. 3 % dioxane Vs apparent molal volume (L_2)

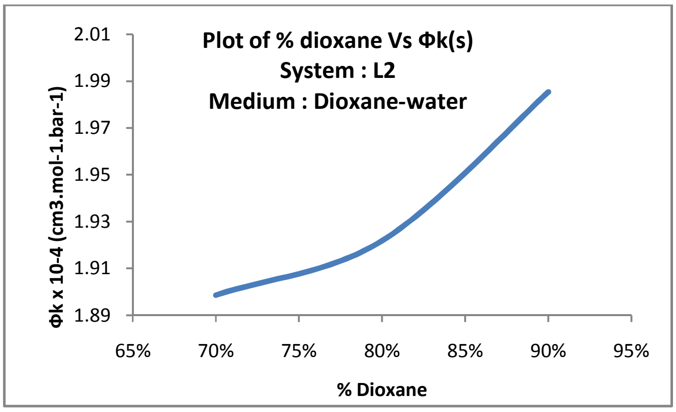

Fig. 4 % dioxane Vs apparent molal compressibility (L_2)

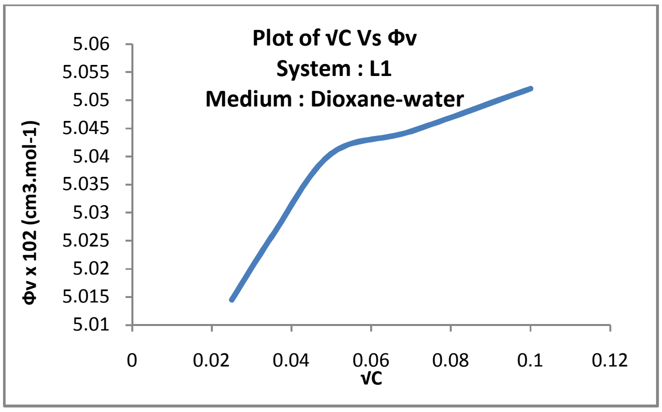

Fig. 5 √C Vs apparent molal volume (L_1)

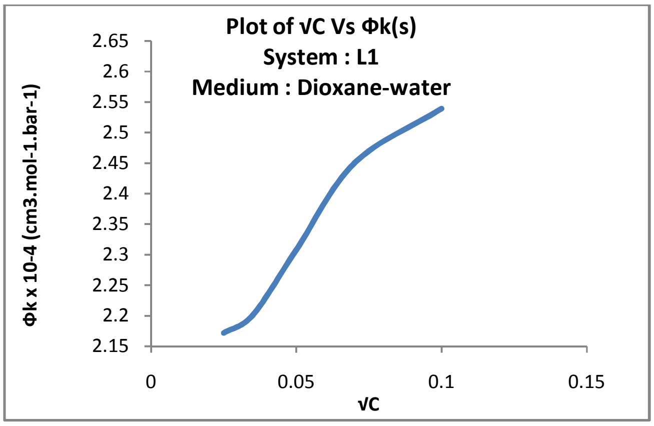

Fig. 6 √C Vs apparent molal compressibility (L_1)

The values of Φ_v and Φ_k have been used to discuss the interaction of unlike molecule of solvents in presence of solute. From Figs. 1-4 values of apparent molal volumes (Φ_v) and apparent molal compressibility (Φ_k) are increased with increase in % dioxane-water mixture of ligand L_1&L_2 irregularly. Tables III and IV showed adiabatic compressibility (β_s) increased with increase in percentages of dioxane-water mixtures. The intermolecular free length (L_f)is found to be insimilar behavior, increase in free length results decrease ultrasonic velocity on the basis of sound propagation in the liquid. These results showed that there is weak solute-solvent interaction.

It could be even concluded from Figs. 5 and 6 that, the apparent molal volume(Φ_v)and apparent molal compressibility (Φ_k)are increased with increase in concentrations of ligand L_1 and ligand L_2.This may be due to the presence of two chlorine group nearer to the hydroxyl group in ligand-L_1 and one chlorine group in ligand-L_2. From Tables I and II, the values of adiabatic compressibility shows that, it decreases with decrease in concentrations of ligand L_1 and vice versa for ligand L_2.The intermolecular free length also observed similar behaviour. This indicates there is weak solute-solvent interaction. The relative association (R_A) and acoustic impedance (Z) are decreases linearly with increase in percentages of dioxane-water mixtures and concentration of ligand-L_1 and L_2. This results showed solute-solvent interaction may occur in the system.

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