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ULTRASONIC STUDY OF ISOXAZOLINE AT DIFFERENT CONCENTRATION IN 70% OF 1, 4-DIOXANE-WATER MIXTURE

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Abstract: The ultrasonic velocity study of the heterocyclic compounds i.e. ultrasonic velocity, adiabatic compressibility, apparent molal volume, apparent molal compressibility have been determined for the synthesized isoxazoline at different concentrations in the dioxane-water mixture by using ultrasonic interferometer at 1 MHz frequency. The variations in acoustical properties with increasing in concentration of the heterocyclic compounds have been used to understand the changes in molecular interactions between solute and solvent to know the structure making and breaking property of solute molecules with increase in concentration of isoxazoline molecules.

Keywords: Adiabatic compressibility, acoustic properties, ultrasonic velocity, apparent molal volume, apparent molal compressibility.

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INTRODUCTION

The nonbonding interactions between two species are called as intermolecular interaction. The intermolecular interaction play important role in providing stability to proteins and various other biological molecules. The three dimensional structure of biopolymer such as proteins, nucleic acids are also due to interaction of hydrogen bonding and hydrophobic group. The molecular interactions are also responsible for the guest- host binding mechanism in enzymes substrate complexes, antigen- antibody complexes and many drug receptors complexes this relationship govern by a rule i. e. molecular recognition of a host by a guest. This type of interaction use in metabolism and immunological response of the body. This information provides strategy for the designing and development of new drugs for the treatment of various diseases. Amino acids are also known as zwitterions contain both acidic and amino groups, they attract each other due to presence of columbic interactions as well as dipole- dipole interactions are also prevalent in biological systems because many building block polymers are polar in natures[1].

The synthetic heterocyclic compounds found their application in various field like antibacterial, antimycobacterial, trypanocidal, anti HIV activity, genotoxic, herbicidal, analgesic, antinflammatory, muscle relaxant, antileishmanial agents, anticonvulsant, anticancer, antimalerial, antifungal and lipid peroxidation inhibitor, antitubercular, hypnotics, anti depressant, antitumoral, anthelmintic, and insecticidal agent[2-7]. Number of important biochemical molecules and drugs obtained from natural resources contains heterocyclic rings. Presence of heterocyclic rings has profound effect on physiological activity of heterocyclic ring containing compounds and has lead to wide variety of modern drugs.

On the other hand isoxazoline-based compounds are known to exhibit a wide range of biological activities such as antibacterial[8], antifungal,[9] anti-tubercular,[10] PPAR a/g agonists,[11] factor Xa inhibitors,[12] including anticancer activity.[13,14] Recently 3,5-disubstituted isoxazolines are reported to possess anticancer activity with apoptosis-inducing ability.[15] In continuation of our efforts on the design of new anticancer agents[16]

Ultrasonic velocity measurement is one of the highly powerful and sensitive method that reveals the nature and strength of intermolecular interactions occurring in the solutions. So in the recent days there is a vast study going on regarding to analyze the intermolecular interaction in solutions, molecular structures by using ultrasonic velocity techniques and some properties such as adiabatic compressibility, apparent molal volume, and apparent molal compressibility. Theses study provides a new avenue for the understanding intermolecular interaction of various solvent with water. Literature survey shows that many researchers have done the acoustical study by the measurement of density and ultrasonic velocity of different aqueous and non-aqueous systems like dioxane, ethanol etc at different temperatures. In view of the importance of these parameters, an attempt is made to determine the density and ultrasonic velocity of isoxazoline in different percentage of dioxane-water mixtures at a particular temperature.

EXPERIMENTAL

The substituted 2-hydroxy isoxazoline have been synthesized by known methods in the laboratory and their structure are confirmed by on the basis of their analytical data. 1, 4-dioxane was purified by Vogel's standard method. The double distilled water is used for solution preparation of solution of metal salt. The solution of isoxazoline was prepared in pure dioxane. The densities of solutions containing different concentration of ligand in absence and in presence of metal ion were measured by using digital density meter (Aton Paar make). The ultrasonic velocity of the solutions were measured by using ultrasonic interferometer having frequency 1MHz (Mittal Enterprises, Model No F-81) .The constant temperature was mentained by circulating water through the double wall measuring cell made up of steel. In the current study we determined the value of adiabatic compressibility (βs), apparent molal volume (ϕv), apparent molal compressibility (ϕk).The apparent molal volume and apparent molal compressibility have been calculated from following equations.

The following isoxazoline are used for ultrasonic study

i) 3-(2-Hydroxy-3, 5-dichlorophenyl)-5-(2, 4-dichloro phenyl) isoxazoline (HDPIB) **L1**

The apparent molal volumes, adiabatic compressibility and apparent molal adiabatic compressibility were determined by using following formulas.

1. Apparent Molal Volume (ϕ_V)

$(\phi_V) = (M / ds) + [(do – ds) x10^3] / m\ do\ ds$ ---- (1)

Whereas M = Molecular weight of Solute.

d_O = Density of a solvent.

ds = Density of solution.

m = molality of the solution.

2. Adiabatic Compressibility (β_o & β_s)

i) For Solvent $\beta_o = 1/Uo^2 d_o$ -----(2)

ii) For solution $\beta_s = 1/Us^2 d_s$ -----(3)

Were U_o and U_s are ultrasonic velocity in the solvent and solution respectively. d_o and d_s are density of the solvent and solute respectively.

β_o and β_s are adiabatic compressibility of the solvent and solution respectively.

3. Apparent Molal adiabatic compressibility (ϕ_{ks})

$$(\phi_{ks}) = \frac{1000(B_s d_o - B_o d_s)}{m\ d_s.d_o} + \frac{B_s.M}{d_s} \quad \text{---------------------- (4)}$$

4. The graphs of ϕ_v Vs √m were plotted. The value of limiting molal volume of the solution ϕ^0_v at m = 0 and slope S_v were calculated using Mason equation.

$\phi_v = \phi^o_v + S_v m^{1/2}$ ---(5)

Where S_v is the slope of the plot which measures solute-solute interaction. ϕ^o_v measures solute-solvent interaction at infinite dilution.

5. The graphs of ϕ_{ks} Vs √m were plotted. The value of limiting molal adiabatic compressibility ϕ^o_{ks} of the solute at m = 0 and slope S_k were calculated by employing following equation.

$\phi_{ks} = \phi^o_{ks} + S_k\, m^{1/2}$ --(6)

Where S_k is the slope of the plot, which measure solute-solute interaction. ϕ^o_{ks} is the measures of solute-solvent interaction at infinite dilution.

RESULT AND DISCUSSION

The present density measurement study shows that the partial molal volume (ϕ_v) for ligand are negative. This indicates weak solute-solvent interactions with increase in concentration of the ligand, the partial molal volume is found to be increased this suggested that the solute-solvent interaction are slightly increased. At higher concentration (m = 0.006), ligand shows positive value of partial molal volume indicating strong solute-solvent interaction. This might be due to electrostriction of the ligand molecules by the solvent molecules.

The positive and higher value of slope S_v of ϕ_v Vs √m plot for the ligand and ligand + Cu (II) ion systems shows the presence of strong solute-solute interaction in presence of Cu (II) ion suggesting stable complex formation. The limiting apparent partial molal volumes ϕ^0_v are determined by extrapolating the straight line to m = 0. It is called as partial molal volume at infinite dilution or zero concentration, where solute-solute interactions are absent. The negative value of ϕ^0_v value indicates absence of solute- solvent interaction; this may be due to zero concentration of the ligands in the solution. The higher values of S_v than ϕ^0_v absence and presence of Cu (II) ions suggests stronger solute- solute interactions than solute- solvent interaction.

The ϕ_k value in the absence of Cu (II) ions are decreased with increase in concentration of the ligand this suggested that there is loss in compressibility and the solute- solvent interactions are increase the ϕ_k value of ligand presence of Cu (II) ions are initially increased and then decreased with increase in concentration ligand this irregular trend in variation of ϕ_k values indicates continuous change in strength of solute- solvent interaction due to stereo chemical changes occurring in the solution.

Table 1 (ϕ_V) and (ϕ_{ks}) values in 70%dioxane –water mixture

System: - (HDPI-B) L_1

Temp = 30 ± 0.1°C Ultrasonic frequency = 1 MHz

Sr. No.	Concentration of ligand $m/10^{-3}$ mol.kg^{-1}	$\phi_{ks}/10^{-2}$ m^3 mol^{-1} pa^{-1}	ϕ_V /10^{-6}m^{3}mol^{-1}
1	1.00	4.89511	-1499.87
2	2.00	-1.28877	-428.5290

3	3.00	0.09929	-55.7316
4	4.00	1.7128	-9.1318
5	6.00	-1.5178	57.398

Table 2 (ϕ_V) and (ϕ_{ks}) values in70% dioxane –water mixture

System: - (HDPI-B) L_1+ Cu (II)

Temp = 30 ± 0.1°C Ultrasonic frequency = 1 MHz

Sr. No.	Concentration of ligand m/10^{-3} mol.kg^{-1}	$\phi_{ks}/10^{-2}$ m^3 mol^{-1} pa^{-1}	ϕ_V /$10^{-6}m^3mol^{-1}$
1	1.00	-8.9173	-1127.060
2	2.00	-4.4565	-568.1615
3	3.00	0.5956	-125.587
4	4.00	-4.3980	208.4646
5	6.00	-1.16199	-35.78144

Table 3 ϕ^0_v, ϕ^0_{Ks}, S_v and S_k values for ligand system

Ligand	$\phi^0_v/10^{-6}$ m^3 mol^{-1}	S_v /$10^4kg^{1/2}m^3$ $mol^{-3/2}$	$\phi^0_{Ks}/10^{-12}m^3$ $mol^{-1}Pa^{-1}$	S_k / $kg^{1/2}m^3$ $mol^{-3/2}$ Pa^{-1}
(HDPI-B) L_1	-800	1.25	9.3	-140

Table 4 ϕ^0_v, ϕ^0_{Ks}, S_v and S_k values for ligand + metal system

Ligand	$\phi^0_v/10^{-6}m^3mol^{-1}$	S_v /$10^4kg^{1/2}m^3$ $mol^{-3/2}$	$\phi^0_{Ks}/10^{-12}m^3$ $mol^{-1}Pa^{-1}$	S_k / $kg^{1/2}m^3$ $mol^{-3/2}Pa^{-1}$
(HDPI-B) L_1+ Cu(II)	-2060	3.50	-8.7	148

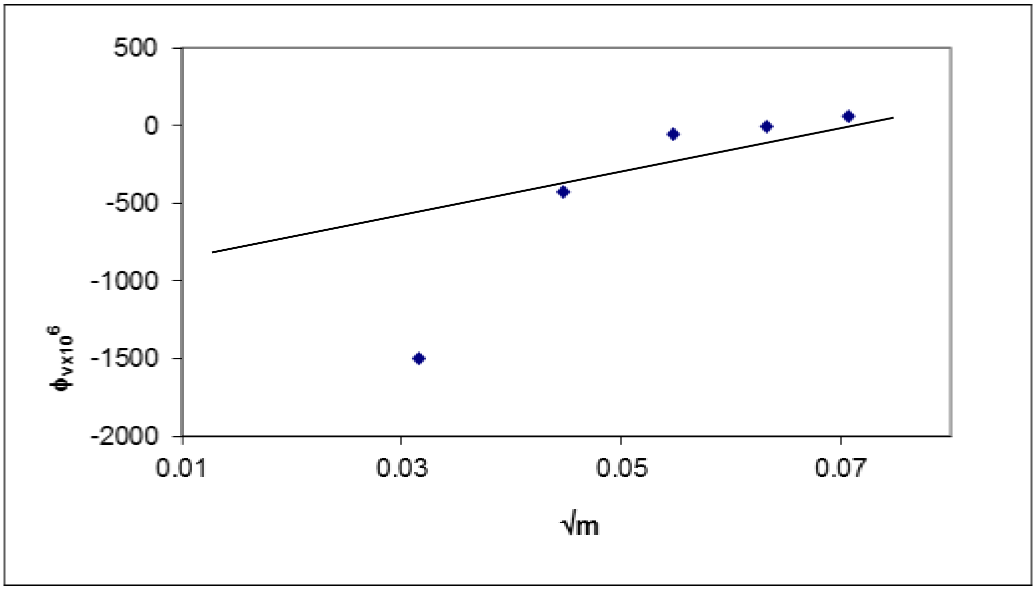

Fig. 1 system -(HDPI-B) L_1 (ϕ_V) Vs √m

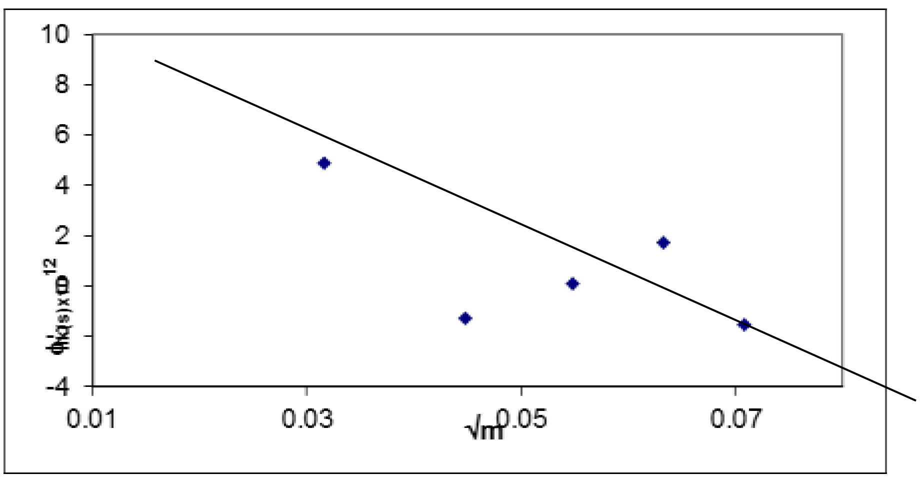

Fig. 2 system -HDPI-L_1 (ϕ_{ks}) Vs √m

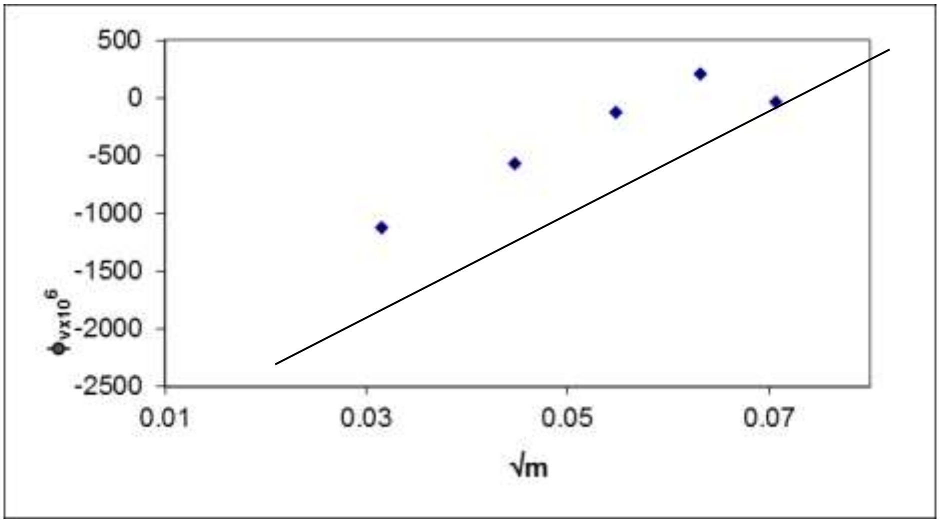

Fig. 3 system -(HDPI-B) L_1-Cu (II) (ϕ_V) Vs √m

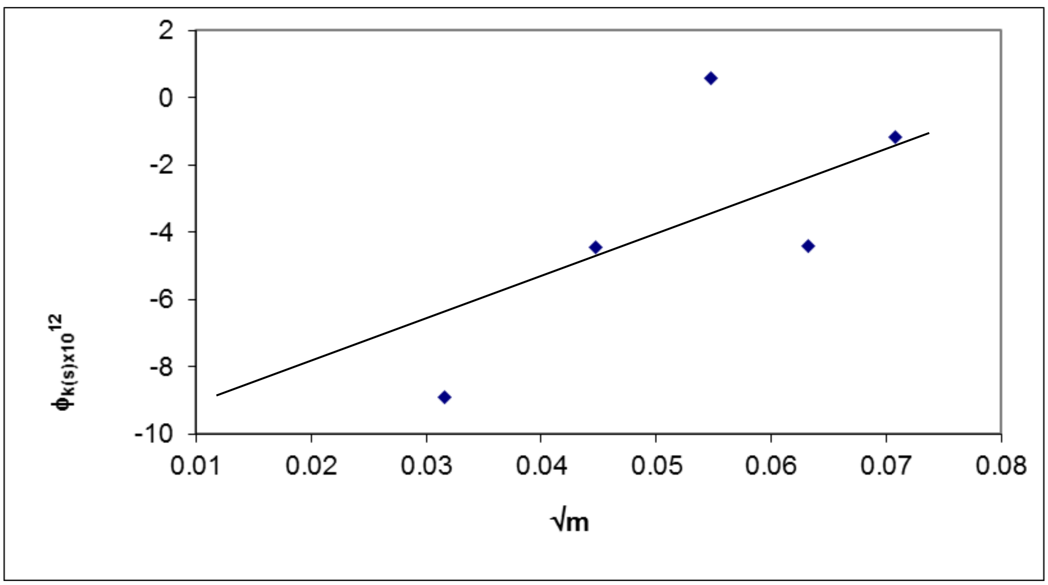

Fig. 4 system -(HDPI-B) L_1- Cu (II) (ϕ_{ks}) Vs √m

CONCLUSION:

The substituted 2-hydroxy isoxazoline has been synthesized from chalcone derivatives, by reacting with hydroxyl amine hydrochloride in presence of solvent ethanol. Acoustical properties were measured for this heterocyclic compound in 1,4-dioxane solvent at constant temperature. The results from the graph shows that there is a is good solute- solvent interaction present between the solute and solvent molecule.

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