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Molecular interaction study of substituted azomethine drugs by ultrasonic technique

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ABSTRACT

The present investigation, deals with the study of some acoustical parameters, including ultrasonic velocity (U), adiabatic compressibility (β s), partial molal volume (φ v), apparent molal compressibility (φ k), solvation number (Sn) of substituted azomethine in 70% DMF+water mixture at 300K. The results thus obtained helps to predict, the effect of concentration of solute on different acoustical parameters inbinary mixture at a constant temperature.

Keywords: Substituted azomethine, ultrasonic velocity, density, acoustic parameter.

INTRODUCTION

Azomethines are of considerable interest because of their chemistry and potentially beneficial biological activities. Azomethine can form a new class of drugs through mechanisms of immune potentiation and therapeutic potential. The complex combination of azomethine with metallic ions are a class of compounds with the most interesting properties both from the point of view of the chemical behavior and the biological one.

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 association. The sound wave propagates through liquids. The frequency of waves more than 20KHz are known as ultrasonic waves.Ultrasonic studies in aqueous solutions of various drugs yield information about the nature of molecular interactions. Voleisines has been studied the structural properties of solution by measuring ultrasonic velocity[1-2]. Ultrasonic study of polysterene solution was also reported[3-4].The thermodynamic parameter, volumetric, acoustic, optical and viscometric properties of binary mixtures of drugswas reported[5-7]. The influence of ultrasonic energy on seed germination was studied byKrishna[8]. Ultrasonic studies in aqueous solutions of various drugs yield information about the nature of molecular interactions as observed by several researchers [9-18].Literature survey shows the study of acoustical properties of substitutedthiopyrimidines and substituted oxoimidazoline drugs in 70% (DMF–water) mixtureat different concentrations of ligands are reported[19].

MATERIALS AND METHODS

The substituted azomethine drug were synthesized by standard method[20]. All chemicals of AR grade were used. Freshly prepared doubly distilled water was used. The densities of pure solvent and solutions of various concentrations were measured at constant temperature using a precalibrated bicapilary pyknometer. All the weighings were made on one pan digital balance (petit balance AD_50B) with an accuracy of \pm (0.001)gm. The

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speed of sound waves was obtained by using variable path crystal interferrometer (Mittal Enterprises, Model MX-3) with accuracy of $\pm (0.03)$ % and frequency 1MHz.

In the present work, a steel cell fitted with a quartz crystal of variable frequency was employed. The instrument was calibrated by measuring ultrasonic velocity of water at 25°C. 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 $\pm (0.1)^{\circ}$ C. The different substituted azomethine ligand used for present work as-



 $\begin{array}{l} L_1 = 2,2' \cdot (benzene-1,2diylbis[nitrilo(1E)eth-1-yl-1-ylidene] \cdot dibenzene-1,4 \cdot diol \\ L_2 = 2,2' \cdot (benzene-1,2diylbis[nitrilo(1E)eth-1-ylidene) bis(4 \cdot nitrophenol) \\ L_3 = 4'4 \cdot (benzene-1,2diylbis[nitrilo(1E)eth-1-yl-1-ylidene] bis(2,-chloro phenol) \\ L_4 = 4'4 \cdot (benzene-1,2diylbis[nitrilo(1E)eth-1-yl-1-ylidene] bis(2,6dichloro phenol) \\ \end{array}$

Calculation:

The sound velocity of each ligand was measured in the concentration range of 1×10^{-1} to 6.25 x 10^{-4} M in 70% (DMF+water) mixture.

Wavelength of ultrasonic wave is calculated using relation.

 $2D = \lambda$ (1)

Where λ is wave length and D is distance in mm.

The ultrasonic velocity is calculated by using relation.

Ultrasonic velocity (U) = λ x Frequency x 10³(2)

Some acoustical parameters have been calculated using the standard relations. The adiabatic compressibility (β s) of solvent and solution are calculated by using equations

Adiabatic compressibility solution (βs) = 1/Us²x ds(3)

Adiabatic compressibility solvent ($\beta 0$) = 1/ $U_0^2 \times d_0 \dots (4)$

Where, U_0 , Us are ultrasonic velocity, d_0 and ds are density in solvent and solution respectively.

The apparent molal volume (φv) and apparent molal adiabatic compressibilities ($\varphi k(s)$ of substituted azomethines in solutions are determined respectively, from density (ds) and adiabatic compressibility(βs) of solution using the equations

 $\varphi v = (M/ds) + [(do-ds) \ 103] / mdsdo....(5)$

And

 $\varphi k(s) = [1000(\beta sdo-\beta ods) / mdsdo] + (\beta s M / ds) \dots (6)$

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Where, m is the molality and M is the molecular weight of solute

βo and βs are the adiabatic compressibilities of solvent and solution respectively.

Solvation number (Sn) = $\varphi \kappa / \beta 0x$ (M/d0)(7)

Where, K is Jacobson's constant24is calculated by using relation

 $K = (93.875 + 0.375 xT) x10^{-8}....(8)$

Where T is temperature at which experiment is carried out.

Table 1: Ultrasonic velocity, density, adiabatic compressibility (β_s), apparent molal volume (φv), apparent molal compressibility (φk),
solvation number (Sn) at different concentration of substituted azomethines in 70% DMF solvent at 300K	

Conc. (m) Moles lit ⁻¹	Density (ds) Kg m ⁻³	Ultrasonic Velocity (Us) m s ⁻¹	Adiabatic Compressibility (βS) x10 ⁻⁹ m ² N ⁻¹	Apparent molal volume (\u03c6v) m ³ mole ⁻¹	Apparent molal compressibility (φk)x10 ⁻¹⁰ m ² N ⁻¹	Solvation number (Sn)		
L1								
0.01	974.84	875.6	1.3355	0.2795	4.6283	0.6450		
0.005	973.61	855.2	1.5423	0.4597	5.0352	0.7114		
0.0025	970.81	825.6	1.6332	0.4632	5.4868	0.7753		
0.00125	969.00	785.6	1.7205	0.3309	6.0663	0.8571		
0.000625	967.66	741.6	1.7945	0.3643	6.4520	0.9117		
0.01	979.45	859.6	1.3821	0.5351	6.0781	0.7440		
0.005	977.81	838.4	1.4563	0.9200	6.5771	0.8051		
0.0025	975.83	801.6	1.5945	1.4746	6.6065	0.8087		
0.00125	973.67	763.2	1.7697	2.1451	6.7599	0.8275		
0.000625	970.81	740.4	1.8725	3.1388	6.8305	0.8361		
L3								
0.01	983.24	841.2	1.4352	0.6725	6.0398	0.7769		
0.005	981.67	805.6	1.5614	1.2104	6.1345	0.7891		
0.0025	980.15	781.2	1.6725	2.1583	6.2429	0.8031		
0.00125	978.98	742.4	1.8532	3.9103	6.4034	0.8237		
0.000625	977.29	705.6	2.0514	6.6399	6.6574	0.8564		
L4								
0.01	985.93	815.2	1.5255	0.9188	7.0624	0.7781		
0.005	984.88	785.6	1.6425	1.7336	7.1922	0.7924		
0.0025	983.53	757.2	1.7705	3.1988	7.2824	0.8024		
0.00125	981.84	715.2	1.9936	5.7210	7.4864	0.8229		
0.000625	980.32	700.4	2.0761	10.2171	7.5335	0.8301		



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The experimental data obtained is represented table-1. It is observed that ultrasonic velocity decreases with decrease in concentration for all systems (Fig1), indicates that, there is significant interaction between the ion and solvent molecules. The substituent which increase the electron density on ring have high ultrasonic velocity than ring deactivating substituents. The Fig.2 indicates adiabatic compressibility increase with decrease in concentration of solution may be due to association of ligand molecule in the solution by weak solute-solute interactions. It is also found that apparent molal volume increases with decrease in concentration in all systems due strong intermolecular interaction. Shown in fig-3, at lower concentration of all systems in 70% of (DMF+water) mixture (Fig.4), showing weak electrostatic attractive force in the vicinity of ions causing electrostatic solvation of ions. Because of weak solute-solvent interaction, (fig-5) solvation number(Sn) increase with decrease in concentration of ligands,

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