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Ultrasonic investigation and molecular interaction studies in substituted oxoimidazoline drugs solution at different concentrations

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ABSTRACT

The study of interaction between solute-solute and solute-solvent interaction of substituted imidazolinone in 70% (DMF+water) solvents by measuring ultrasonic velocity and density in different concentration of solute in the range ($1x10^{-2}$ M to $6x10^{-4}$ M) in 70% of solvent has done. In the present investigation, different acoustical parameters, such as ultrasonic velocity (U), adiabatic compressibility (βs), partial molal volume (φv), intermolecular free length (Lf), apparent molal compressibility (φκ), specific acoustic impedance (Z), relative association (RA), solvation number (Sn) of substituted imidazolinone in 70% of DMF+water mixture at 298K have been studied. With the help of experimental data,the effect of concentration of solute on different acoustical parameters in DMF-water mixtures at a constant temperature and deviation of acoustical parameter from the ideality has been studied.

Key words Substituted oximidazolinone, ultrasonic velocity, Density, acoustic parameter.

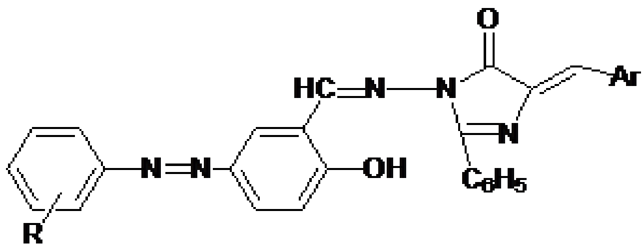
INTRODUCTION

The sound wave propagates through liquids. The frequency of waves more than 20 KHz are known as ultrasonic waves. In the recent year, an ultrasonic wave has acquired the status of an important tool for the study of structure and properties of matter in basic science. In medical science, the waves are being used for medical diagnosis

[1], for the detection of bone fractures, cancer tumors and physiotherapy, bloodless surgery, cardiology[2,3], gynecology etc. Ultrasonic techniques are best suited for physico-chemical studies of a system. 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. Ultrasonic techniques reveal very weak intermolecular interactions due to its useful wavelength range.

In recent years, ultrasonic velocity and absorption studies in case of electrolyte solutions have led to new insight into the process of ion-association and complex-formation[4,5]. Number of workers such as Sonar[6], Thirumarun[7], Armstrong and Johnson[8], Kanhekar[9], Agrawal and Deosarkar[10] have made ultrasonic study of electrolytic solutions and discussed about the variation of ultrasonic velocity with ion concentration. Most of the ultrasonic work in non-aqueous systems possesses an interpretation of solute-solvent interactions[11]. Solvation numbers have been obtained from the study of non-aqueous solutions by Dudhe[12],Harish Kumar And Deepika[13]. Tadkalkar[14] have studied molecular velocity and molecular compressibility from ultrasonic data. Miss Pankati etal[15] have investigated the adiabatic compressibility and hydration numbers of amino acids in water solvent and water-dioxane mixtures. Sawalakhe etal[16-17] have studied the adiabatic compressibility and apparent molar volume of diketones, pyrazoles and pyrazolines in water-dioxane, water-tetrahydrofuran and water-acetone mixtures. Ikhe[18] have studied the adiabatic compressibility and apparent molal volume of some antibiotic drugs. Wadekar [19] have investigated the adiabatic compressibility, apparent molal compressibility and other parameters of ligands with Fe(III) metal. Kachare[20],Praharaj and Dondge [21-22] have studied the apparent molal volumes of alcohols in aqueous solutions at different temperatures. The effect of temperature on acoustical parameters and molecular interactions in liquid mixtures, salt solutions has been studied by many workers[23-24]. But compressibilities and apparent molal volumes of substituted imidazolinone in DMF have not been studied so far.

In the present communication the measurement of ultrasonic velocity and density in different concentration of solute in 70% of solvent has done. ,also the present attempt is made to study the other acoustical parameters such as adiabatic compressibility (βs), partial molal volume (φv), intermolecular free length (Lf), apparent molal compressibility (φκ), specific acoustic impedance (Z), relative association (RA), solvation number (Sn) of substituted imidazolinone in 70% of (DMF+water) mixture at different concentrations of ligand. The different substituted oxoimidazoline ligand used for present work as-



L_A: R = -3-Chloro

L_B: R = -H

L_C: R = -4-Bromo

L_D: R = -2-Bromo

L_E: R = -4-methoxy

LA = 1-[2-hydroxy-5-(3-chloro phenyl azo) benzylidene amino]-2-phenyl-4-benzylidene- 5-oxoimidazoline
LB = 1-[2-hydroxy-5-(phenyl azo) benzylidene amino]-2-phenyl-4-benzylidene- 5-oxoimidazoline
LC = 1-[2-hydroxy-5-(4-bromo phenyl azo) benzylidene amino]-2-phenyl-4- benzylidene- 5-oxoimidazoline
LD = 1-[2-hydroxy-5-(2- bromo phenyl azo) benzylidene amino]-2-phenyl-4-benzylidene- 5-oxoimidazoline
LE = 1-[2-hydroxy-5-(4-methoxy phenyl azo) benzylidene amino]-2-phenyl-4-benzylidene- 5-oxoimidazoline

Experimental

The ligands of which physical parameters is to be explore are synthesized by using reported protocol[25]. The DMF of AR grade was 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 + 0.001 gm. The speed of sound waves was obtained by using variable path crystal interferrometer (Mittal Enterprises, Model MX-3) with accuracy of + 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 25oC. 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 + 0.1oC.

Calculation

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

wavelength of ultrasonic wave is calculated using relation.

$$2D = \lambda \qquad \text{…………. (1)}$$

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 10^3 ……….(2)

Some acoustical parameters have been calculated using the standard relations.

The adiabatic compressibility (βs) of solvent and solution are calculated by using equations

Adiabatic compressibility solution (βs) = $1/ Us^2 x\ ds$ ……... (3)

Adiabatic compressibility solvent (β_0) = $1/ U_0^2\ x\ d_0$ ……… (4)

Acoustic impedance (Z) = Us x ds ……. (5)

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

d_0 and ds are density of solvent and solution respectively

The apparent molal volume (ϕ_v) and apparent molal adiabatic compressibilities ($\phi_{k(s)}$) of substituted imidazolinone in solutions are determined respectively, from density (d_s) and adiabatic compressibility(β_s) of solution using the equations

$\phi_v = (M/d_s) + [(d_o-d_s)\ 10^3] / md_sd_o$ .... (6)

And
$\phi_{k(s)} = [1000(\beta_s d_o-\beta_o d_s) / md_sd_o] + (\beta_s\ M / d_s)$ ……… (7)

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

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

Intermolecular free length (Lf) = $K\sqrt{\beta s}$ ………… (8)

Relative association (RA) = $(ds /d0)\ x\ (U0 /Us)^{1/3}$ ....(9)

Solvation number (Sn) = $\varphi^{\kappa} / \beta 0x\ (M/ d0)$ …….. (10)

Where, K is Jacobson's constant[26] is calculated by using relation

$K=(93.875+0.375xT)x10^{-8}$ ……….. (11)

where T is temperature at which experiment is carried out.

RESULTS AND DISCUSSION

Table1: Ultrasonic velocity, density, adiabatic compressibility (βS), Specific acoustic impedance (Z), Intermolecular free length (Lf) of different concentration of substituted oxoimidazoline in 70% DMF solvent at 298K

Conc. (m) Moles lit-1	Density (ds) Kg m-3	Ultrasonic Velocity(Us) m s-1	Adiabatic Compressibility (βS) x10-9 m2N-1	Inter molecular free length (Lf) x10-11 m	Specific acoustic impedance (Z) x105 kg m-2s-1
L_A in 70% (DMF +water) solvent					
0.01	1016.8	906.8	1.1960	7.1112	9.2203
0.005	1014.4	870.8	1.3000	7.4140	8.8333
0.0025	1012.8	835.2	1.4154	7.7361	8.4589
0.00125	1011.4	795.2	1.5636	8.1308	8.0426
0.000625	1010.5	771.6	1.6621	8.3833	7.7970
L_B in 70% (DMF +water) solvent					
0.01	1022.9	848.4	1.3582	7.5780	8.6782
0.005	1021.4	816.4	1.4689	7.8808	8.3387
0.0025	1020.9	814.8	1.4754	7.8982	8.3182
0.00125	1019.8	806.0	1.5094	7.9888	8.2195
0.000625	1017.4	802.8	1.5250	8.0301	8.1676
L_C in 70% (DMF +water) solvent					
0.01	1013.8	834.0	1.4181	7.7434	8.4550
0.005	1012.8	828.0	1.4401	7.8034	8.3859
0.0025	1011.9	821.2	1.4654	7.8715	8.3097
0.00125	1011.2	811.2	1.5028	7.9713	8.2028
0.000625	1010.4	796.0	1.5620	8.1267	8.0427
L_D in 70% (DMF +water) solvent					
0.01	1022.5	830.0	1.4196	7.7475	8.4867
0.005	1021.8	822.8	1.4455	7.8180	8.4073
0.0025	1021.1	818.0	1.4636	7.8666	8.3525
0.00125	1020.6	808.0	1.5008	7.9659	8.2464
0.000625	1019.9	804.8	1.5137	8.0003	8.2081
L_E in 70% (DMF +water) solvent					
0.01	1021.5	821.6	1.4502	7.8306	8.3926
0.005	1020.8	816.0	1.4712	7.8870	8.3297
0.0025	1020.1	810.8	1.4911	7.9403	8.2709
0.00125	1019.4	800.0	1.5327	8.0503	8.1552
0.000625	1018.8	788.0	1.5807	8.1753	8.0281

Table-2: Concentration (m), relative association (RA), apparent molal compressibility (φκ), apparent molal volume (φv), solvation number (Sn) of different concentration of substituted oxoimidazoline at 70% (DMF+ water) solvent at 298K

Conc (m) Moles/lit	Apparent molal volume (φv) m3mole-1	Apparent molal compressibility (φk)x10−10 m2N-1	Relative association (RA)	Solvation number (Sn)
		L_A in 70% (DMF +water) solvent		
0.01	2.4648	6.2318	0.9873	0.6549
0.005	4.7095	6.7769	0.9983	0.7122
0.0025	9.1229	7.3821	1.0107	0.7758
0.00125	17.7247	8.1586	1.0260	0.8575
0.000625	34.7762	8.6764	1.0354	0.9118
		L_B in 70% (DMF +water) solvent		
0.01	2.5531	6.5969	1.0155	0.7441
0.005	4.9811	7.1379	1.0271	0.8051
0.0025	9.8785	7.1697	1.0272	0.8087
0.00125	19.3881	7.3359	1.0298	0.8275
0.000625	37.1543	7.4125	1.0288	0.8361
		L_C in 70% (DMF +water) solvent		
0.01	2.5273	8.0341	1.0122	0.7775
0.005	4.9540	8.1596	1.0136	0.7896
0.0025	9.7262	8.3033	1.0155	0.8035
0.00125	19.1689	8.5161	1.0190	0.8241
0.000625	37.6874	8.8527	1.0246	0.8567
		L_D in 70% (DMF +water) solvent		
0.01	2.9564	8.0425	1.0225	0.7783
0.005	5.8449	8.1901	1.0248	0.7926
0.0025	11.5535	8.2927	1.0261	0.8025
0.00125	22.9119	8.5042	1.0298	0.8231
0.000625	45.2761	8.5782	1.0305	0.8301
		L_E in 70% (DMF +water) solvent		
0.01	2.6536	7.4967	1.0250	0.7950
0.005	5.2449	7.6057	1.0266	0.8065
0.0025	10.3651	7.7094	1.0281	0.8175
0.00125	20.4798	7.9254	1.0320	0.8404
0.000625	40.5292	8.1747	1.0366	0.8669

Fig. 1 comperative Plots of Ultrasonic velocity Us in m s^{-1} Vs Concentration (Mole/lit.) in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E

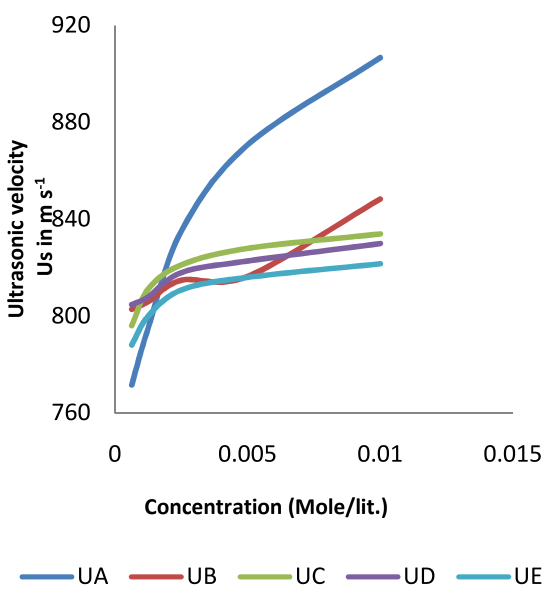


Fig. 2 comperative Plots of adiabatic compressibility (β_S) x10^{-9} m^{2}N^{-1} Vs Concentration (Mole/lit.) in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .

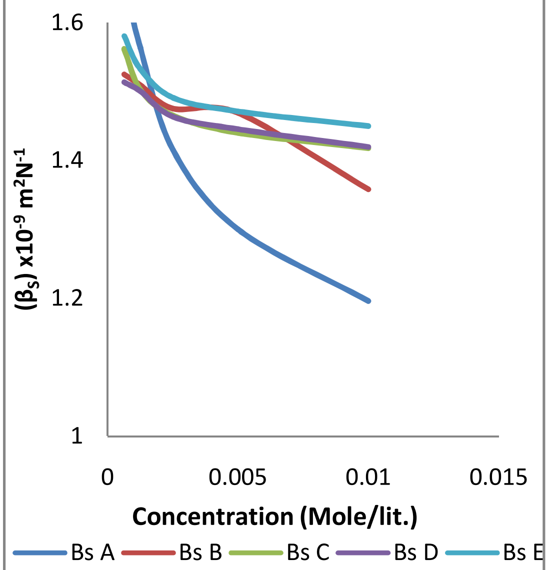


Fig. 3 Comperative Plots of Inter molecular free length (Lf) x10^{-11} mVs Concentration (Mole/lit.) in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .

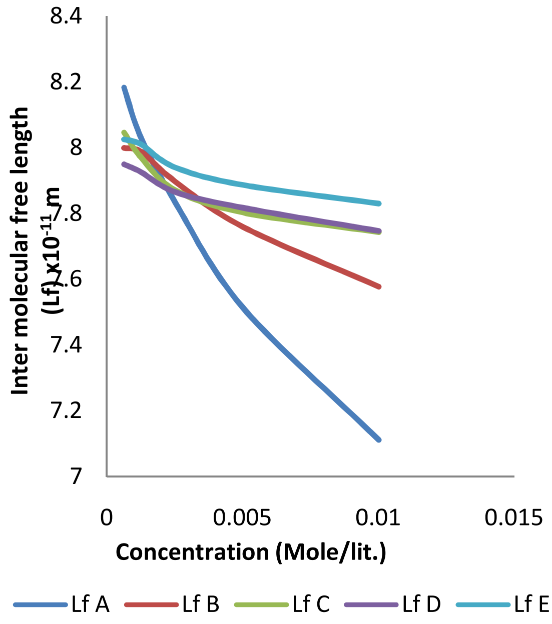


Fig. 4 Comperative Plots of Specific acoustic impedance (Z) x10^5 kg m^{-2}s^{-1} Vs Concentration (Mole/lit.) in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .

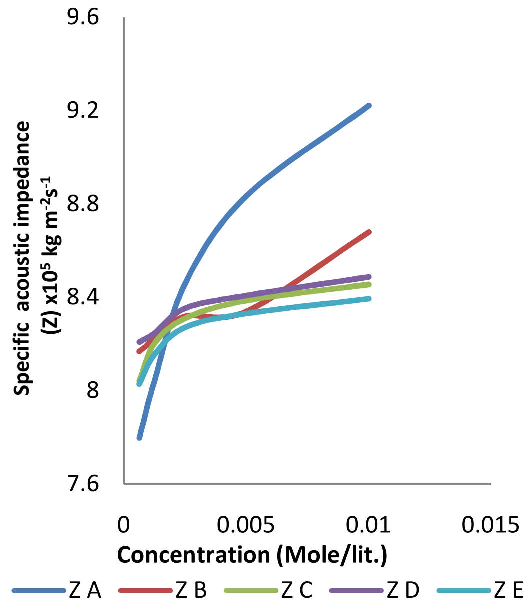


Fig.5 Comperative Plot of Apparent molal volume (φv) m^{3}mole^{-1} Vrs concentration in mole/lit in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .

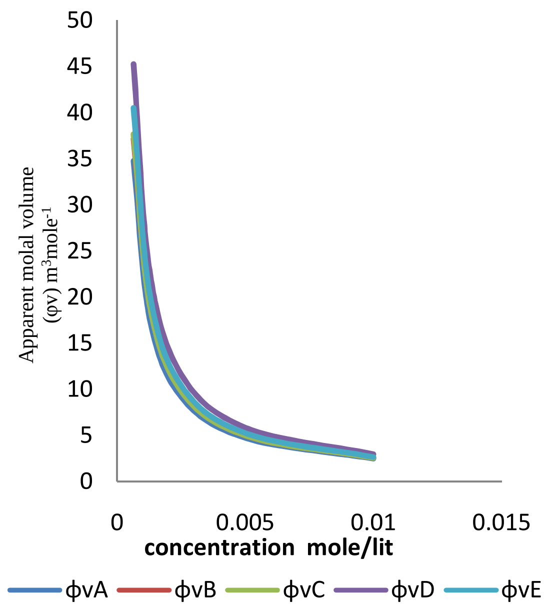


Fig.6 Comperative plot of Apparent molal compressibility (φk)x10^{-10} m^{2}N^{-1} Vrs concentration in mole/lit in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .

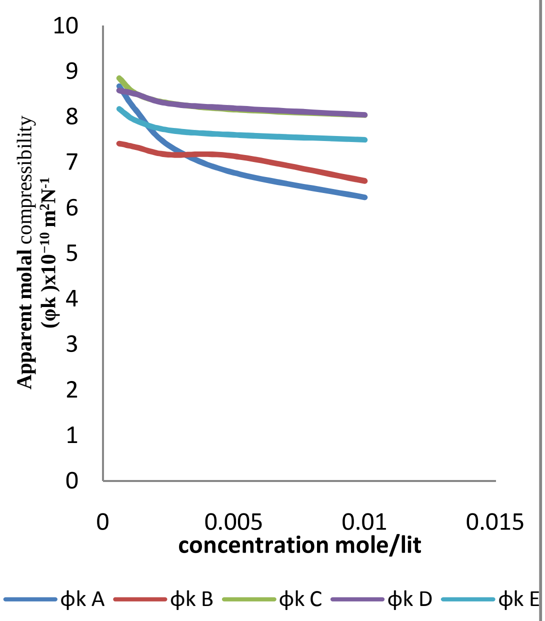


Fig. 7 Comperative Plots of Relative association (RA) Vs Concentration (Mole/lit.) in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .

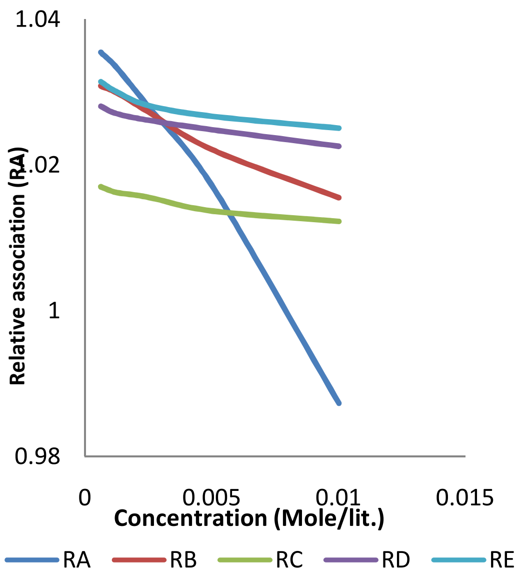
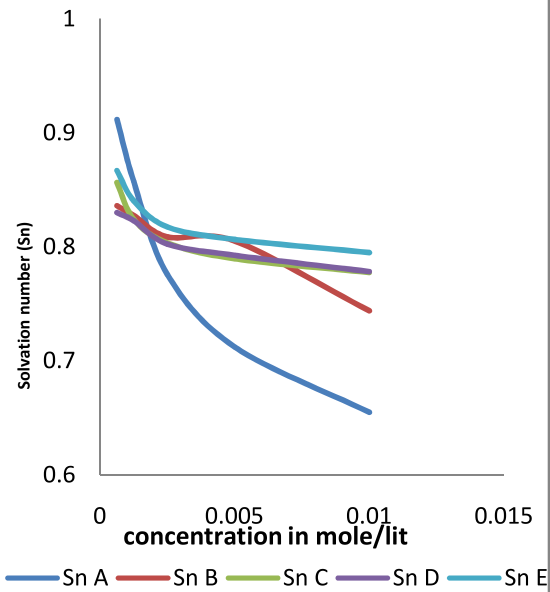


Fig.8 Comperative Plot of solvation number (Sn) Vrs concentration in mole/lit in 70% DMF solvent for L_A, L_B, L_C, L_D, L_E .



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RESULTS AND DISCUSSION

From table 1, it is found that ultrasonic velocity decreases with decrease in concentration for all systems(fig 1) .This indicates that, there is significant interaction between ion and solvent molecules suggesting a structure promoting behavior of the added electrolyte. The substituent which decrease the electron density on oxoimidazoline ring have high ultrasonic velocity than ring activating substituents. The increase of adiabetic compressibility with decrease of concentration of solution may be due to the dispersion of solvent molecules around ions supporting weak ion-solvent interactions (fig. 2). Adiabatic compressibility is more in case of bulky and less polar substituents. It was found that, intermolecular free length increases linearly on decreasing the concentration of substituted 5-imidazolinone in different solution of DMF+water mixture (fig. 3). The intermolecular free length increase due to greater force of interaction between solute and solvent by forming hydrogen bonding and less interaction between two solute molecules. The value of specific acoustic impedance (Z) decreases with decrease in concentration for all substituted imidazolinone in 70% solutions of (DMF+water) mixture (fig.4).

From table 2, it is observed that apparent molal volume increases with decrease in concentration in all systems indicates the existence of stronge ion-solvent interaction(fig.5). the value of apparent molal volume is high in case of more polar substituent than less polar substituents. The value of apparent molal compressibility increases with decrease in concentration of all systems in 70% of (DMF+water) mixture (fig.6), showing weak electrostatic attractive force in the vicinity of ions causing electrostatic salvation of ions. Compressibility is more in case of bulky substituents. The value of relative association increases with decrease in concentration in all systems (fig.7). It is found that there is weak interaction between solute and solvent. Relative association is more in case of bulky and more poalar substituents. The solvation number increase with decrease in concentration due to weak solute-solvent interaction (fig.8). The Solvation number in all system increases with decrease in concentration solute indicates the large solvent molecule are present around the solute molecule which increase the solubility of solute.

CONCLUSION

In the present study mentions the experimental data for ultrasonic velocity, density and at 298K for all substituted Oxoimidazoline drugs in (DMF-water) mixture. From the experimental data it is concluded that there is a weak solute- solvent and solvent- solvent interaction between substituted oxoimidazoline ,water and DMF molecules.

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