Studies in Acoustical Properties of Subsitituted Quinoline Pyrimidines Drugs In 70% (DMF–Water) Mixture

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Abstract : The study of interaction between solute-solute and solute-solvent interaction of substituted Quinoline pyrimidines 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% solvent has done. In the present investigation, different acoustical parameters, such as ultrasonic velocity (U), adiabatic compressibility (βs), partial molal volume (φv), apparent molal compressibility (φκ), solvation number (Sn) of substituted Quinoline pyrimidines in 70% DMF+water mixture at 300K 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.

Keywords: Substituted Quinoline pyrimidines, ultrasonic velocity, Density, acoustic parameter.

INTRODUCTION

In the recent years much interest has been focused on the study of the Quinoline ring system because of its potential pharmacological activities. pyrimidines and aminopyrimidines[1, 2] are also broadly found in bioorganic and medicinal chemistry with applications in drug discovery and developments. They are reported to possess broad spectrum of biological activities such as antibacterial[3], fungicidal[4], insecticidal[5], antihypertensive[6], tranquilizing[7], analgesic[8], antidiabetic[9] etc. In light of above biologicaactivities, it is worthwhile to synthesis thiopyrimidine derivatives[10] which may have some good biological activities.

The measurement of acoustic properties contributes to the understanding of the physicochemical behavior of the binary and multi-component liquid mixtures. Excess properties of liquid systems, such as molal volumes, are required for testing the theories of solutions, development of separation techniques and equipment and for other industrial applications. Thus, a study of physical properties data on the binary mixture containing DMF and Water have attracted considerable interest in the literature[11, 12].

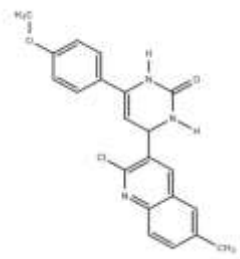
The sound wave propagates through liquids. The frequency of waves more than 20 KHz are known as ultrasonic waves. In the recent year, an ultrasonic wave has acquired the status of an important tool for the study of structure and properties of matter in basic science.

In medical science, the waves are being used for medical diagnosis[13], for the detection of bone fractures, cancer tumors and physiotherapy, bloodless surgery, cardiology[14], 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.

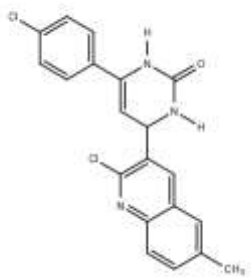
In recent years, ultrasonic velocity and absorption studies in case of electrolyte solutions have led to new insight into the process of ion-association and complex-formation[15, 16]. Solvation numbers have been obtained from the study of non-aqueous solutions[17]. Many workers studied adiabatic compressibility, apparent molal compressibility and other parameters of ligands in binary solvent[18-20]. Also the study of apparent molal volumes of alcohols in aqueous solutions at different temperatures is carried out[21, 22]. But compressibilities and apparent molal volumes of substituted Quinoline pyrimidines 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% solvent has done. Also the present attempt is made to study the other acoustical parameters such as adiabatic compressibility (βs), partial molal volume (φv), apparent molal compressibility (φκ), and solvation number (Sn) of substituted Quinoline pyrimidines in 70% of (DMF + water) mixture at different concentrations of ligand. The different substituted Quinoline pyrimidines ligand used for present work as-

L_1: *4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-methoxyphenyl)-3, 4- dihydropyrimidin-2(1H)-one*



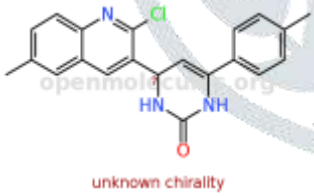
L_2: *4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-chlorophenyl)-3, 4- dihydropyrimidin-2(1H)-one*



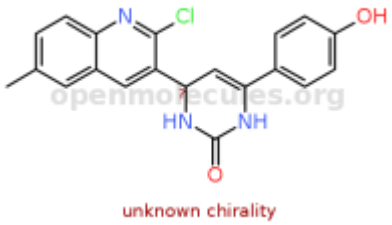
L3: ***4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-fluorophenyl)-3, 4- dihydropyrimidin-2(1H)-one***

L_4- *4-(2-Chloro-6-methylquinolin-3-yl)-6-phenyl-3, 4-dihydropyrimidin-2(1H)-one*

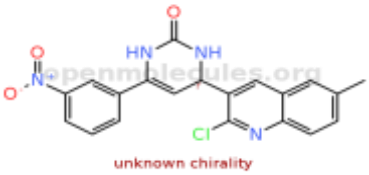
L_5* - *4-(2-Chloro-6-methylquinolin-3-yl)-6-(p-tolyl)-3, 4- dihydropyrimidin-2(1H)-one



L_6* - *4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-hydroxyphenyl)-3, 4- dihydropyrimidin-2(1H)-one



L_7 _ 4-(2-Chloro-6-methylquinolin-3-yl)-6-(3-nitrophenyl)-3, 4- dihydropyrimidin-2(1H)-one



EXPERIMENTAL

The substituted thiopyrimidines of which physical parameters are to be explore were synthesized by using reported protocol [23]. All chemicals of AR grade were used. Experiment was carried out in freshly prepared doubly distilled water. 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 27ºC. 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 each ligand was measured in the concentration range of 1×10^{-1} to 6.25×10^{-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 $(U) = \lambda \times \text{Frequency} \times 10^3$ …. (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 $(\beta s) = 1/ U_s^2 \times d_s$ ... (3)

Adiabatic compressibility solvent $(\beta_0) = 1/ U_0^2 \times d_0$ ... (4)

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 ($\varphi_{k(s)}$) of substituted thiopyrimidines in solutions are determined respectively, from density (d_s) and adiabatic compressibility(β_s) of solution using the equations

$\varphi_v = (M/d_s) + [(d_o-d_s)\, 10^3] / m d_s d_o$ ... (5)

And $\varphi_{k(s)} = [1000(\beta_s d_o - \beta_o d_s) / m d_s d_o] + (\beta_s M / d_s)$ … (6)

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.

Solvation number

$(Sn) = \varphi\kappa / \beta_o \times (M/ d_o)$ … (7)

Where, K is Jacobson's constant[24]is calculated by using relation $K= (93.875+0.375xT) \times 10^{-8}$ … (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 thiopyrimidines in 70% DMF solvent at 300K.

Conc. (m) Moles lit^{-1}	Density (ds) Kg m^{-3}	Ultrasonic Velocity(Us) m s^{-1}	Adiabatic Compressibility (β_s) $x10^{-9}$ $m2N^{-1}$	Apparent molal volume (φv) m^3mole^{-1}	Apparent molal compressibility (φk)$x10^{-10}$ m^2N^{-1}	Solvation number (Sn)
L1						
0.01	1126.3	895.2	1.1079	4.8600	4.2099	0.6026
0.005	1125.3	861.6	1.1970	9.6769	4.5529	0.6517
0.0025	1125.2	839.2	1.2619	19.3452	4.8024	0.6874
0.00125	1124.1	830.0	1.2913	38.5000	4.9155	0.7036
0.000625	1122.9	827.2	1.3014	76.5827	4.9545	0.7092
L2						
0.01	1225.3	871.6	1.0742	7.2456	4.4644	0.5845
0.005	1224.3	860.0	1.1043	14.4592	4.5907	0.6010
0.0025	1224.2	836.4	1.1676	28.9121	4.8565	0.6358
0.00125	1223.1	828.0	1.1925	57.6825	4.9610	0.6495
0.000625	1222.1	825.6	1.2004	115.106	4.9944	0.6538
L3						
0.01	1224.6	863.2	1.0959	7.2344	4.5553	0.5964
0.005	1222.4	852.4	1.1259	14.3979	4.6812	0.6128
0.0025	1219.2	833.2	1.1814	28.5874	4.9146	0.6434
0.00125	1218.5	824.4	1.2075	57.0830	5.0240	0.6577
0.000625	1217.9	822.4	1.2140	114.008	5.0513	0.6613
L4						
0.01	1253.2	860.0	1.0789	8.5143	4.9828	0.5876
0.005	1250.2	843.6	1.1239	16.9324	5.1926	0.6123
0.0025	1243.3	831.2	1.1641	33.4133	5.3800	0.6344
0.00125	1240.2	822.0	1.1933	66.4130	5.5160	0.6504
0.000625	1239.6	820.4	1.1985	132.664	5.5404	0.6533

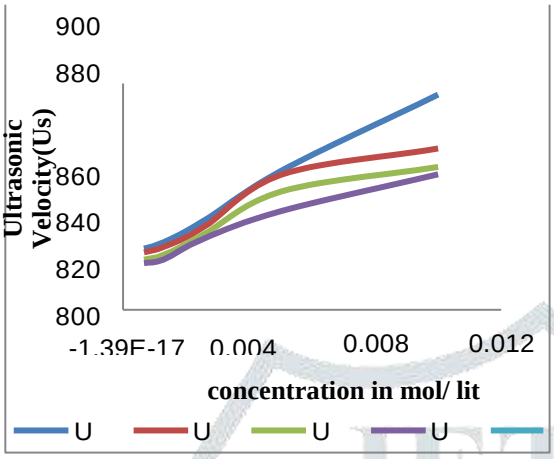


Fig-1: Plot of Ultrasonic Velocity(Us) m s^{-1} Vrs concentration (mole/lit) in 70% DMF solvent

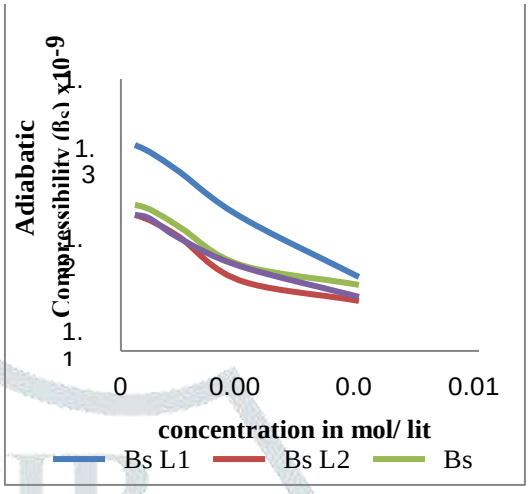


Fig-2: Plot of Adiabatic Compressibility (βS) $x10^{-9}$ m^2N^{-1} Vrs concentration (mole/lit) in 70% DMF solvent

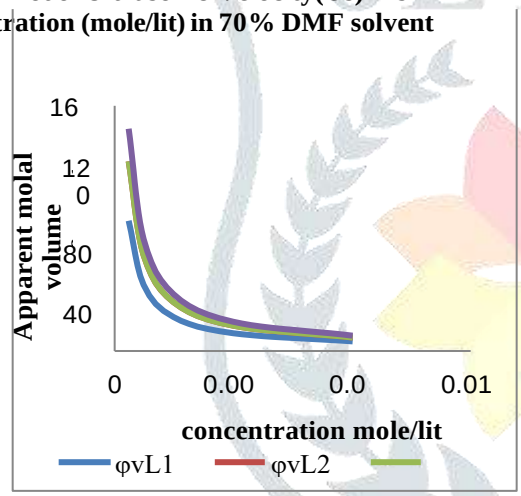


Fig-3: Plot of Apparent molal volume (φv)m^3mole^{-1} Vrs concentration in mole/lit in 70% DMF solvent

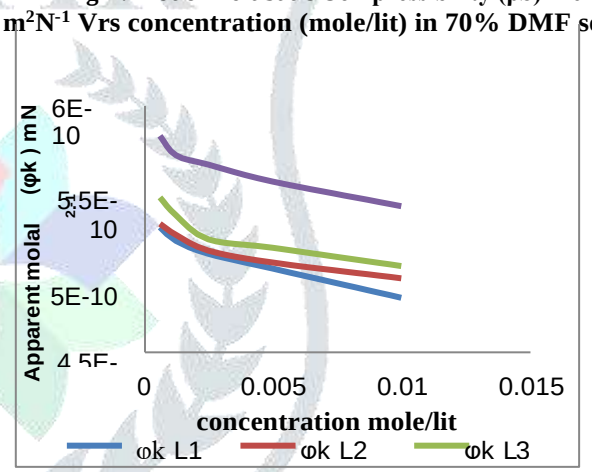


Fig-4: plot ofApparent molal compressibility (φk) m^2N^- Vrs concentration in mole/lit in 70% DMF solvent.

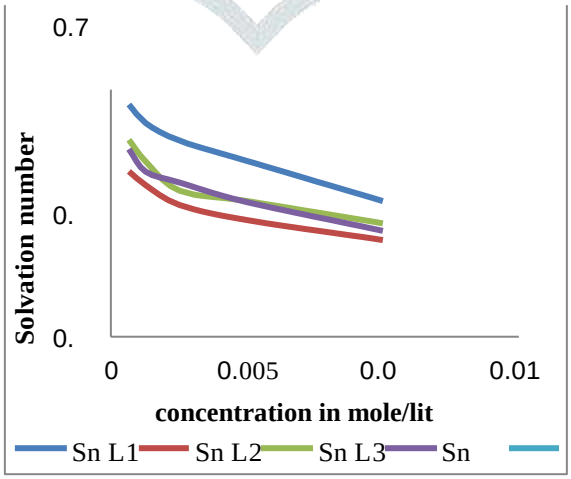


Fig-5: Plot of solvation number (Sn) Vrs concentration in mole/lit in 70% DMF solvent.

RESULT AND DISCUSSION

Observation table-1, gives the idea about different types of variation in acoustical parameters of ligands due to different types of substitution on thiopyrimidines structure. It is found that ultrasonic velocity decreases with decrease in concentration for all systems (Fig1) .This indicates that, there is significant interaction between ion and solvent molecules, suggesting a structure promoting behavior of the added electrolyte. The substituent which increase the electron density on pyrimidines ring have high ultrasonic velocity than ring deactivating substituents. The increase of adiabatic compressibility with decrease in concentration of solution may be due to association of ligand molecule in the solution by weak solute- solute interactions (Fig.2). Adiabatic compressibility is more in case of small and less polar substituents. Apparent molal volume increases with decrease in concentration in all systems indicates the existence of strong intermolecular interaction. From fig-3, at lower concentration its value is very high. The value of apparent molal volume is high in case of more polar substituent than less polar substituent. The value of apparent molal compressibility increases with decrease in 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. Compressibility is more in case of bulky and more polar substituent. The solvation number increase with decrease in concentration due to weak solute-solvent interaction (Fig.5). Also indicates solute molecule has more space for their movement in solution.

CONCLUSION

Present study mentions the experimental data of ultrasonic velocity(U), density(d), adiabatic compressibility (βs), partial molal volume (φv), apparent molal compressibility ($\varphi \kappa$), solvation number (Sn) for all substituted thiopyrimidine drugs in (DMF-water) mixture at 300K. From the experimental data it is concluded that there is a weak solute- solvent and solvent-solvent interaction between substituted thiopyrimidine, water and DMF molecules. And variation in acoustical parameter is due to the different substitution in the structure of ligand molecules.

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