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

Dr. A. S. Shrirao
Assistant Professor in Chemistry
Ghulam Nabi Azad Arts, Commerce & Science College Barshitakli Dist-Akola India

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 been 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 aminopyrimidines1-2 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 antibacterial3, fungicidal4, insecticidal5, antihypertensive6, tranquilizing7, analgesic8, antidiabetic9 etc. In light of above biolgicaactivities, it is worthwhile to synthesis thiopyrimidine derivatives10 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 on the binary mixture containing DMF and Water have attracted considerable interest in the literature11, 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 diagnosis13, for the detection of bone fractures, cancer tumors and physiotherapy, bloodless surgery, cardiology14, 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-formation15, 16. Solvation numbers have been obtained from the study of non-aqueous solutions17. Many workers studied adiabatic compressibility, apparent molal compressibility and other parameters of ligands in binary solvent18-20. Also the study of apparent molal volumes of alcohols in aqueous solutions at different temperatures is carried out21, 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- 

L₄: 4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-methoxyphenyl)-3, 4- dihydropyrimidin-2(1H)-one

[Image of the molecule]
L₂: 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

L₄: 4-(2-Chloro-6-methylquinolin-3-yl)-6-phenyl-3, 4-dihydropyrimidin-2(1H)-one

L₅: 4-(2-Chloro-6-methylquinolin-3-yl)-6-(p-tolyl)-3, 4-dihydropyrimidin-2(1H)-one

L₆: 4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-hydroxyphenyl)-3, 4-dihydropyrimidin-2(1H)-one
EXPERIMENTAL

The substituted thiopyrimidines of which physical parameters are to be explore were synthesized by using reported protocol. 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 capillary 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 interferometer (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 27°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 ±0.1°C.

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

Wavelength of ultrasonic wave is calculated using relation.

\[ 2D = \lambda \]  
Where \( \lambda \) is wave length and D is distance in mm.

The ultrasonic velocity is calculated by using relation.

\[ U = \lambda \times \text{Frequency} \times 10^3 \]  
Some acoustical parameters have been calculated using the standard relations. The adiabatic compressibility (\( \beta_s \)) of solvent and solution are calculated by using equations

\[ \text{Adiabatic compressibility of solution} (\beta_s) = 1/ U s^2 \times ds \]  
\[ \text{Adiabatic compressibility of solvent} (\beta_s) = 1/ U s^0 \times d_s \]

Where, \( U_s \) and \( U_s^0 \) are ultrasonic velocity in solvent and solution respectively. \( d_s \) and \( d_s^0 \) are density of solvent and solution respectively.

The apparent molal volume (\( \psi_v \)) and apparent molal adiabatic compressibilities (\( \psi_{k(s)} \)) of substituted thiopyrimidines in solutions are determined respectively, from density (\( d_s \)) and adiabatic compressibility (\( \beta_s \)) of solution using the equations

\[ \psi_v = (M/d_s) + [(d_{so(6)} - d_s) 10^3] / \text{md}_{ds} \]  
And \( \psi_{k(s)} = [10000(\beta_s/d_{so(6)} - \beta_s/d_s) / \text{md}_{ds}] + (\beta_s \times M / d_s) \)

Where, m is the molality and M is the molecular weight of solute. \( \beta_s \) and \( \beta_v \) are the adiabatic compressibilities of solvent and solution respectively.

Solvation number

\[ (Sn) = \psi_k / \beta_v \times (\text{M} / d_s) \]

Where, \( K \) is Jacobson’s constant, \( \psi_k \) is calculated by using relation \( K = (93.875+0.375xT) \times 10^{-8} \)

Where \( T \) is temperature at which experiment is carried out.
Table 1: Ultrasonic velocity, density, adiabatic compressibility ($\beta_s$), Apparent molal volume ($\varphi_v$), Apparent molal compressibility ($\varphi_k$), Solvation number ($S_n$) at different concentration of substituted thiopyrimidines in 70% DMF solvent at 300K.

<table>
<thead>
<tr>
<th>Conc. (m) Moles lit$^{-1}$</th>
<th>Density (ds) Kg m$^{-3}$</th>
<th>Ultrasonic Velocity (Us) m s$^{-1}$</th>
<th>Adiabatic Compressibility ($\beta_s$) x10$^{-9}$ m$^2$N$^{-1}$</th>
<th>Apparent molal volume ($\varphi_v$) m$^3$mole$^{-1}$</th>
<th>Apparent molal compressibility ($\varphi_k$) x10$^{-10}$ m$^2$N$^{-1}$</th>
<th>Solvation number ($S_n$)</th>
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Fig 1: Plot of Ultrasonic Velocity ($U_s$) m s$^{-1}$ Vrs concentration (mole/lit) in 70% DMF solvent

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

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

Fig 4: Plot of Apparent molal compressibility ($\phi_k$) m$^2$N$^{-1}$ 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 (ov), apparent molal compressibility (oc), 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 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.

REFERENCES
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