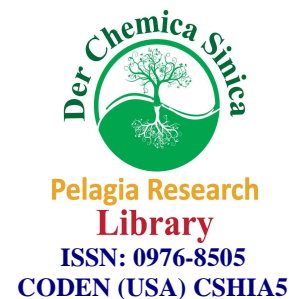




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### Molecular interaction study of substituted thiopyrimidines in the binary mixture

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#### ABSTRACT

*In the present investigation, some important acoustical parameters, such as ultrasonic velocity( $U$ ), intermolecular free length( $L_f$ ), specific acoustic impedance( $Z$ ), relative association( $RA$ ) of substituted thiopyrimidines in 70% of 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 and deviation of acoustical parameter with the change in concentration has been studied.*

**Key words:** Substituted thiopyrimidines, ultrasonic velocity, Density, acoustic parameter.

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#### INTRODUCTION

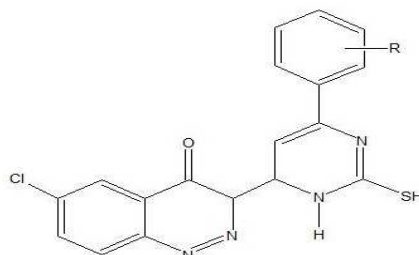
Pyrimidine moiety is an important class of nitrogen containing heterocycles[1] and is widely used as a key building block for pharmaceutical agents. Its derivatives exhibit antibacterial, antifungal[2], analgesic[3], calcium antagonist[4], anti-inflammatory[5] and anti-tumor activity[6]. In addition, several marine natural products with interesting biological activities containing pyrimidine core have recently been isolated[7]. Most notably among these are the batzelladine alkaloids A and B which inhibit the binding of HIV envelope protein gp-120 to human CD<sub>4</sub> cells.

In continued quest of new anti-inflammatory agents we herein report the ultrasonic study of certain thiopyrimidine derivatives. 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. 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[8-9]. Number of workers have made ultrasonic study of electrolytic solutions and discussed about the variation of ultrasonic velocity with ion concentration[10-14]. Most of the ultrasonic work in non-aqueous systems possesses an interpretation of solute-solvent interactions[15-16]. The effect of temperature on acoustical parameters and molecular interactions in liquid mixtures, salt solutions has been

studied by many workers[17-18]. But compressibilities and apparent molal volumes of substituted thiopyrimidins 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 intermolecular free length (Lf), specific acoustic impedance (Z), relative association (RA), of substituted thiopyrimidine in 70% of (DMF+water) mixture at different concentrations of ligand. The different substituted thiopyrimidine ligand used for present work as-



L <sub>1</sub> : R = -H
L <sub>2</sub> : R = -2-Chloro
L <sub>3</sub> : R = -3-Chloro
L <sub>4</sub> : R = -3-Bromo

L<sub>1</sub>: 6-chloro-3-(2-mercapto-6-phenyl-3,4-dihydropyrimidin-4-yl)cinnolin-4(3H)one  
 L<sub>2</sub>: 6-chloro-3-(6-(2-chlorophenyl)-2-mercapto-3,4-dihydropyrimidin-4-yl) cinnolin-4(3H) one  
 L<sub>3</sub>: 6-chloro-3-(6-(3-chlorophenyl)-2-mercapto-3,4-dihydropyrimidin-4-yl) cinnolin-4(3H) one  
 L<sub>4</sub>: 3-(6-(3-bromophenyl)-2-mercapto-3,4-dihydropyrimidin-4-yl)-6-chlorocinnolin- 4(3H)one

### Experimental

The ligand synthesis is carried out by known method [19-20]. All chemicals of AR grade were used. The densities of pure solvent and solutions of various concentrations were measured at constant temperature using a precalibrated bicapillary pycnometer. All the weighings were made on one pan digital balance (petit balance AD\_50B) with an accuracy of  $\pm 0.001$  gm. The speed of sound waves was obtained by using variable path crystal interferometer (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 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  $\pm 0.1^\circ\text{C}$ .

### Calculation

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

wavelength of ultrasonic wave is calculated using relation.

$$2D = \lambda \quad (1)$$

Where  $\lambda$  is wave length and D is distance in mm.

The ultrasonic velocity is calculated by using relation.

$$\text{Ultrasonic velocity (U)} = \lambda \times \text{Frequency} \times 10^3 \quad (2)$$

Some acoustical parameters have been calculated using the standard relations.

The adiabatic compressibility ( $\beta_s$ ) of solvent and solution are calculated by using equations

$$\text{Adiabatic compressibility solution } (\beta_s) = 1/ U_s^2 \times ds \quad (3)$$

$$\text{Adiabatic compressibility solvent } (\beta_0) = 1/ U_0^2 \times d_0 \quad (4)$$

$$\text{Acoustic impedance (Z)} = U_s \times ds \quad (5)$$

Where,  $U_0$ ,  $d_0$ ,  $\beta_0$  and  $U_s$ ,  $ds$ ,  $\beta_s$  are ultrasonic velocity, density and adiabatic compressibilities of solvent and solution respectively.

$$\text{Intermolecular free length (Lf)} = K\sqrt{\beta_s} \quad (6)$$

$$\text{Relative association (RA)} = (\text{ds} / \text{d0}) \times (\text{U0} / \text{Us})^{1/3} \quad (7)$$

Where, K is Jacobson's constant[20] is calculated by using relation

$$K = (93.875 + 0.375 \times T) \times 10^{-8} \quad (8)$$

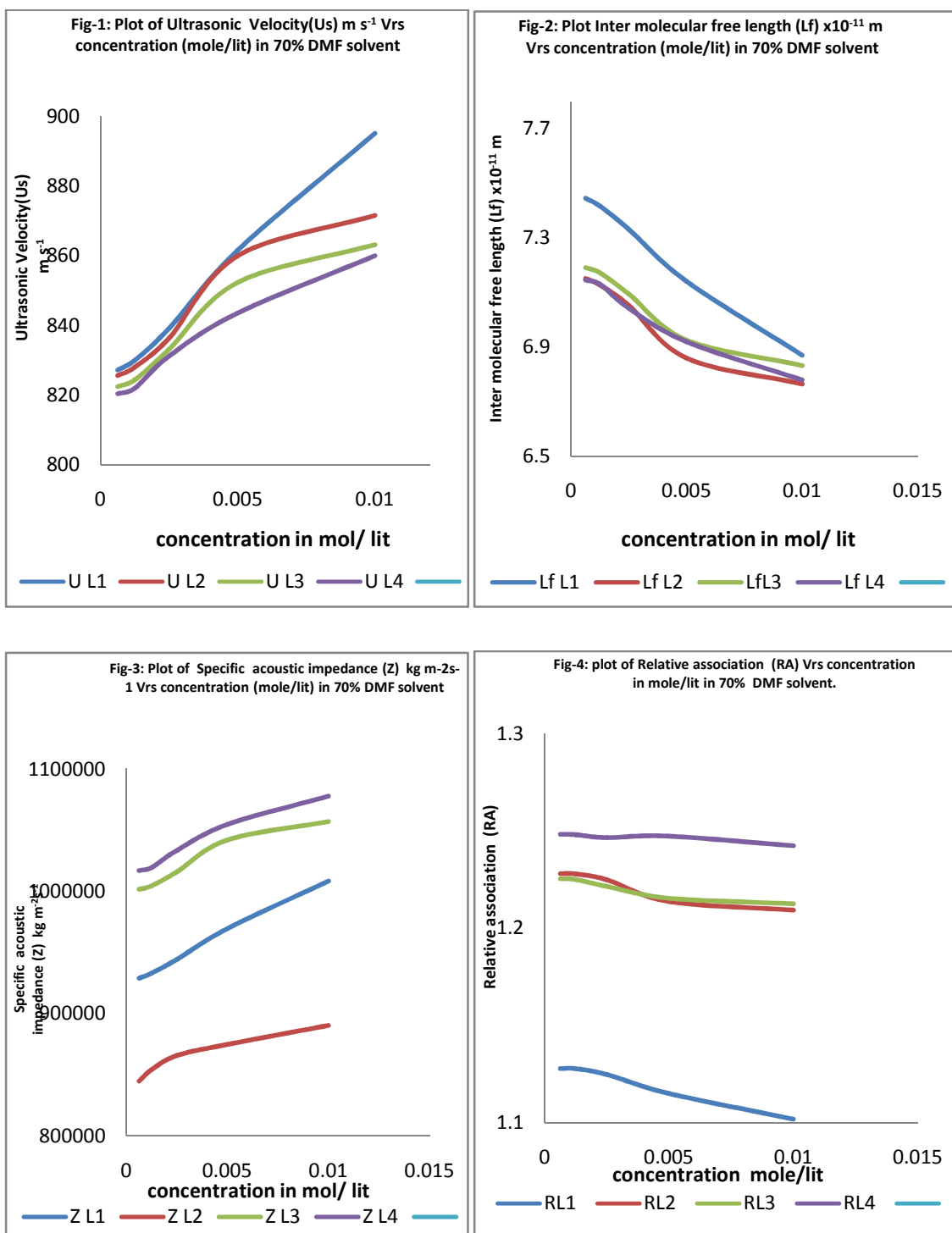
where T is temperature at which experiment is carried out.

**Table-1: Ultrasonic velocity, density, Inter molecular free length (Lf), Specific acoustic impedance (Z), relative association (RA), at different concentration of substituted thiopyrimidines at 70% (DMF+ water) solvent at 300K**

Conc (m) Moles/lit	Density (ds) Kg m <sup>-3</sup>	Ultrasonic Velocity(Us) m s <sup>-1</sup>	Inter molecular free length (Lf) x10 <sup>-11</sup> m	Specific acoustic impedance (Z) x10 <sup>5</sup> kg m <sup>-2</sup> s <sup>-1</sup>	Relative association (RA)
<b>L<sub>1</sub></b>					
0.01	1126.3	895.2	6.8692	10.0826	1.1017
0.005	1125.3	861.6	7.1403	9.6955	1.1149
0.0025	1125.2	839.2	7.3312	9.4426	1.1246
0.00125	1124.1	830.0	7.4161	9.3300	1.1276
0.000625	1122.9	827.2	7.4451	9.2886	1.1277
<b>L<sub>2</sub></b>					
0.01	1225.3	871.6	6.7642	10.6797	1.2093
0.005	1224.3	860.0	6.8582	10.5289	1.2137
0.0025	1224.2	836.4	7.0520	10.2392	1.2249
0.00125	1223.1	828.0	7.1268	10.1272	1.2279
0.000625	1222.1	825.6	7.1504	10.0896	1.2281
<b>L<sub>3</sub></b>					
0.01	1224.6	863.2	6.8320	10.5707	1.2125
0.005	1222.4	852.4	6.9248	10.4197	1.2154
0.0025	1219.2	833.2	7.0936	10.1583	1.2215
0.00125	1218.5	824.4	7.1714	10.0453	1.2251
0.000625	1217.9	822.4	7.1906	10.0160	1.2255
<b>L<sub>4</sub></b>					
0.01	1253.2	860.0	6.7787	10.7775	1.2423
0.005	1250.2	843.6	6.9188	10.5466	1.2473
0.0025	1243.3	831.2	7.0414	10.3343	1.2466
0.00125	1240.2	822.0	7.1291	10.1944	1.2481
0.000625	1239.6	820.4	7.1448	10.1696	1.2483

## 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 increase the electron density on thiopyrimidine ring have high ultrasonic velocity than ring deactivating substituents. It was found that, intermolecular free length increases linearly on decreasing the concentration of substituted thiopyrimidine in different solution of DMF+water mixture (fig 2). 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 thiopyrimidine in 70% solutions of (DMF+water) mixture (fig.3). The value of relative association mostly depends on concentration of solute in solution. For higher concentration greater the value of relative association and vice versa. The decrease in concentration, relative association increases in all systems (fig.4). It is found that there is weak interaction between solute and solvent. Relative association is more in case of bulky and more polar substituents.



### CONCLUSION

In the present study mentions the experimental data for ultrasonic velocity, density and at 300K for all substituted thiopyrimidine 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 thiopyrimidine, water and DMF molecules.

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**REFERENCES**

- [1] Patil AD, Kumar NV, Kokke WC, Bean MF, *J.Org.Chem.*, **1995**, 60, 1182.
- [2] Deshmukh MB, Salunkhe SM, Patil DR, *Eur.J.Med.Chem.*, **2009**, 44, 2651
- [3] Sondhi SM, Jain S, Dinodia M, Shukla R, *Bioorg.Med.Chem.*, **2007**, 15, 3334.
- [4] Balkan A, Ertan M, Burgemeister T, *Arch.Pharm.(Weinheim)*, **1992**, 325, 499.
- [5] Sondhi SM, Dinodia, M, Rani, R, Raghbir R, *Ind.J.Chem.*, **2009**, 49b, 273.
- [6] Russowsky D, Canto RFS, Sanches SAA, *Bioorg. Chem.*, **2006**, 34, 173.
- [7] Heys L, Moore CG, Murphy P, *Chem. Soc. Re.*, **2000**, 29, 57.
- [8] Ramteke A, Narwade ML, *Archives of appl. Sci. research*, **2012**, 4(1), 254.
- [9] Sonar AN, *JCPR*. **2011**, 3(4), 485.
- [10] Sonar AN, Pawar NS, *Rasayan J.Chem.*, **2010**, 3(1), 38.
- [11] Thirumarun S, Job K, *Ind. J. Pure & Appli. Phys.*, **2009**, 47, 87.
- [12] Armstrong MM, Johnson AI, *J.acoustical soc.of ind.*, **2011**, 38(4),784.
- [13] Kanhekar SR, Pawar P, *Ind.J.Pure & Appli.Phys.*, **2010**, 48, 95.
- [14] Deosarkar SD, Narwade ML, *Rasayan J.Chem*, **2010**, 3(1),55.
- [15] Syal VK, Baljeet SP, *Ind.J Pure and Appl Phys*, **1999**, 37 (5), 366.
- [16] Tayade RR, Wadekar MP, *JCPR*, **2014**, 6(9), 114.
- [17] Ramarao GV, Sharma V, Ramababu C, *Ind.J.Chem*, **2004**, 43A,752.
- [18] Rohankar PG, Aswar AS, *Ind.J.Chem*, **2002**, 41A (2),312.
- [19] Gaikwad S, Suryavanshi V, *JCPR*, **2012**, 4(3), 1851.
- [20] Sreekanth K, Sravana kumar D, *JCPR*. **2011**,3(4),29-41.