

## Studies on Acoustic Parameters of 1-(4-Hydroxy-6-Methyl Pyrimidino)-3-Methyl Thiocarbamides in 70% Dioxane-Water Mixture at 302<sup>0</sup>k and Frequency 1 Mhz

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### Abstract

*Ultrasonic velocity and density measurements had been carried out for solution of 1-(4-hydroxy-6-methyl pyrimidino)-3-methyl thiocarbamides (HMPMT) in 70% dioxane-water at 302<sup>0</sup>K and frequency 1 MHz. This data have been used to determine various acoustic/thermodynamic parameters viz. adiabatic compressibility, apparent molar compressibility, apparent molar volume, intermolecular free length, relative association and specific acoustic impedance. These properties are used to interpret weak molecular solute-solvent, solute-solute interactions in the system.*

**Key words-** Pyrimidines, Thiocarbamide, Ultrasonic velocity, 70% Dioxane-Water mixture,

### Introduction

Ultrasonic velocity and adsorption studies in case of electrolyte solution have led to new insight into the process of ion association and complex formation<sup>1,2</sup>. Sondawale and Narwade<sup>3</sup> have studied ultrasonic velocity of peptide in binary mixture. Rohankar<sup>4</sup> has investigated the ultrasonic velocity of mono-chloro acetic acid and tri-chloro acetic acid in tetrahydrofuron (THF) and dioxane-water mixture. Ultrasonic velocity of substituted acrylophenones and its complexes in acetone<sup>5</sup> and substituted thiadiazoles and carboxylate at different liquid mixture has been studied<sup>6</sup>. Ikhe and Narwade<sup>7</sup> have studied ultrasonic velocities and densities of isoxazole and pyrazole at 303 K. Naik and Narwade<sup>8</sup> studied metal-ligand stability constant of substituted pyrazole complexes with lanthanide metal ion. The information about the role of metal complexes in biological systems, their concentration and presence in different equilibria is of immense importance. Greshon et. al<sup>9-10</sup> reported that the activity of metal chelates is considerably increased as compared to that of the free metal and ligand alone on their complexation.

Adiabatic compressibilities were used to determine solvation number of ions. For this the wavelength of ultrasonic velocities in solvents and solutions had been evaluated. From these velocities and densities of solutions, adiabatic compressibilities are obtained to calculate solvation number. Pasynski<sup>11</sup> had drawn the conclusion from adiabatic compressibility studies of aqueous electrolytes

solution that the structure of water become more highly coordinated and compacted with the introduction of ions. The absorption of sound by aqueous solutions of electrolytes was studied for frequency, concentration and temperature. Adiabatic compressibility of gelatin solution<sup>12</sup> and aqueous solution of sugar<sup>13</sup> and dicarboxylic and hydroxy carboxylic acids were determined. Asal<sup>14</sup> have determined ultrasonic velocities of hydration and dehydration of polyelectrolyte solutions.

Milerio<sup>15</sup> and coworkers determined the apparent molar volume and adiabatic molar compressibilities of some amino acids in aqueous medium. Hydration numbers were evaluated using partial molar volume and adiabatic compressibility data. This particular field is attracting the attention of several workers, which can be judged from recent publications<sup>16-21</sup> in this filed. Compressibility and apparent molar volumes of many electrolytes in mixed organic solvents were found out earlier.<sup>22-25</sup> But, the compressibility and apparent molar volumes and other acoustic properties of 0.1 M concentration of 1-(4-hydroxy-6-methyl pyrimidino)-3-methyl thiocarbamides in water-dioxane solvent mixture are not studied so far. Therefore, the present work is undertaken to make systematic study of compressibilities and apparent molar volumes of 1-(4-hydroxy-6-methyl pyrimidino)-3-phenyl thiocarbamide at different percentage and also at different concentrations of HMPMT in 70% dioxane-water mixture.

## Experimental

### Materials and Methods:

All weighings were carried out on Mechaniki Zakatasy Precyzynej Gdansk balance made in Poland ( $\pm 0.001$  g). The accuracy of density measurement was within  $\pm 1\%$  K gm-3.

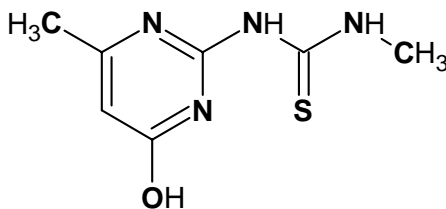
Ultrasonic interferometer from Mittal Enterprises, Model MX-3 with accuracy of  $\pm 0.03\%$  and frequency 1 MHz was used for the measurement of ultrasonic velocities of different solutions.

A special thermostatic arrangement was made during the study. Elite thermostatic water bath was used and temperature variation was maintained within  $\pm 0.1^\circ\text{C}$ .

### Result and Discussion

Adiabatic compressibility ( $\beta$ ), apparent molar volume ( $\phi_v$ ), apparent molar compressibility ( $\beta_k$ ), intermolecular free length ( $L_f$ ), relative association (RA), specific acoustic impedance (Z) and partial molar volume properties directly interferes and reflects the structural interaction of solvent (water/organic solvent) with solute and provide important and valuable information about internal structure, molecular association, complex formation, internal pressure, stability of complexes. Weak molecular interactions can also be detected by this technique. The study of density of solutions at different concentrations is very much important because it helps to calculate the properties like apparent molar volume  $\phi_v$  and apparent molar expansibility  $\beta_k$ .

The Structures of 1-(4-hydroxy-6-methyl pyrimidino)-3-methyl thiocarbamides, is given below.



**1-(4-Hydroxy-6-methylpyrimidino)-3-methylthiocarbamide**

#### Adiabatic compressibility ( $\beta$ ):

Velocity of propagation of mechanical disturbances had to be considered a basic property of liquids in a molecular kinetic theory. A number of theoretical equations relating the ultrasonic velocity and other molecular properties have been established.

By measuring ultrasonic velocity ( $v$ ) and density ( $d$ ) experimentally, the adiabatic compressibility ( $\beta$ ) can be determined by using Laplace's equation.

$$\beta = 1/v^2.d$$

#### Apparent molar compressibility ( $\beta_k$ ):

Apparent molar compressibility ( $\beta_k$ ) is one of important acoustic property which can be determined by measuring density and ultrasonic velocity and depends upon the molality of solution and molecular weight of the solute, by the relation,

$$\beta_k = [1000(\beta_s d_o - \beta_o d_s)/m d_s d_o] + (\beta_s M/ds).$$

#### Apparent molar volume ( $v$ ):

A apparent molar volume did not depend upon ultrasonic velocity but depends upon densities of solution and solvent, molecular weight of solute ( $M$ ) and molality of solution ( $m$ ). It can be determined by the relation,

$$v = [1000(d_o - d_s) /m d_s d_o] + (M/ds).$$

#### Intermolecular free length ( $L_f$ ):

Intermolecular free length ( $L_f$ ) created its own identity in acoustic properties for studying the intermolecular interactions. Hildebrand<sup>26</sup> showed that the center of attraction does not coincide with geometrical center of molecule of liquid as the distance between the centers of attraction is a property extremely difficult to define. The distance between the surfaces of molecules, on the other hand has a clear physical significance so it is used in defining free length.

Intermolecular free length can be determined from adiabatic compressibility ( $\beta$ ) by Jacobson's formula,

$$L_f = K \cdot N \beta$$

### Relative association ( $R_A$ ):

Relative association is a function of ultrasonic velocity and can be obtained by the equation,

$$R_A = ds/ds_0 (V_0/V_s)^{1/3}$$

Where,  $V_0$  and  $V_s$  are ultrasonic velocities in solvent and solution.

### Specific acoustic impedance ( $Z$ ):

Specific acoustic impedance can be obtained from the measurement of ultrasonic velocity and density by formula,

$$Z = v_s \cdot d_s$$

The solute-solvent interactions may be interpreted in terms of acoustic impedance.

### Conclusion

The apparent molal volumes ( $\Delta v$ ) are found to decrease with increase in concentration of solute;  $L_f$  increases on increasing the concentration of solute hence decrease in ultrasonic velocity with the concentration. This indicates that there is a weak interaction between ion and solvent molecules, suggesting a structure non-promoting behaviour of the added solute. The increase of  $\beta_s$  with the concentration may be due to the departure of solvent molecules around the ions<sup>18</sup> due to weak ion-solvent interactions. The increase of  $R_A$  with concentration suggests that solvation of ions predominates over the breaking up of the solvent aggregate on addition of solutes. Acoustic impedance ( $Z$ ) decreases with increase in concentration. It is concluded that the molecular interactions are present between the solute and solvent mixture and solute-solvent interactions are more favorable than other interactions shows in Table-I and Fig-I to Fig-IV.

Table-I

Conc (M)	N C	Us (m sec-1)	Ds (Kg m-3)	s x10-10 (Pa-1)	v (m3mol-1)	k x 10-10 (m3mol-1 Pa-1)	Lf (A°)	RA	Z x 106 (Kg m-2 sec-1)
0.1	0.301	1403.3	994.0	4.340	0.2251	-0.8314	0.01228	1.0001	1.3867
0.08	0.264	1400.6	992.7	4.362	0.2443	-0.0297	0.01232	0.9993	1.4821
0.06	0.230	1395.0	993.1	4.393	0.2471	1.7133	0.01237	1.0010	1.4672
0.04	0.185	1388.1	992.2	4.436	0.2861	9.6603	0.01243	1.0015	1.4694
0.02	0.126	1388.1	992.0	4.440	0.3670	12.0650	0.01244	1.0015	1.4685

Acoustic parameters at different concentration of ligand HMPMT in 70% Dioxane-water.

Temp. =  $29 \pm 0.1^\circ\text{C}$       Ultrasonic Frequency = 1 MHz

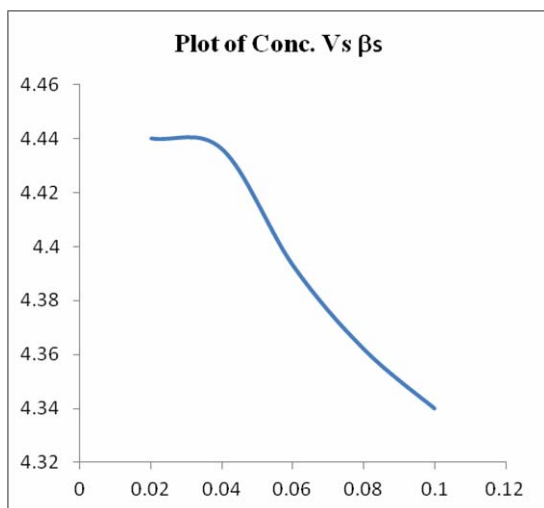


Figure 1

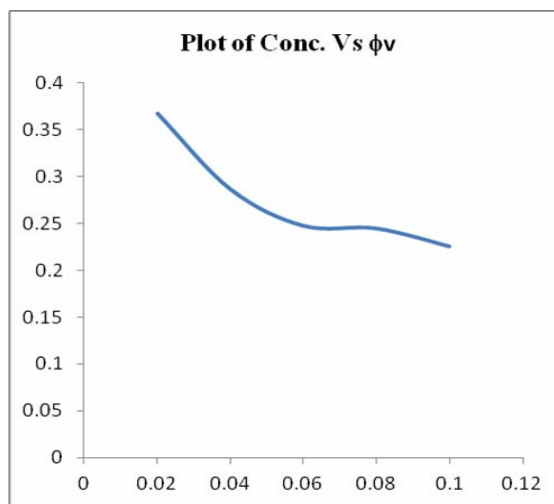


Figure 2

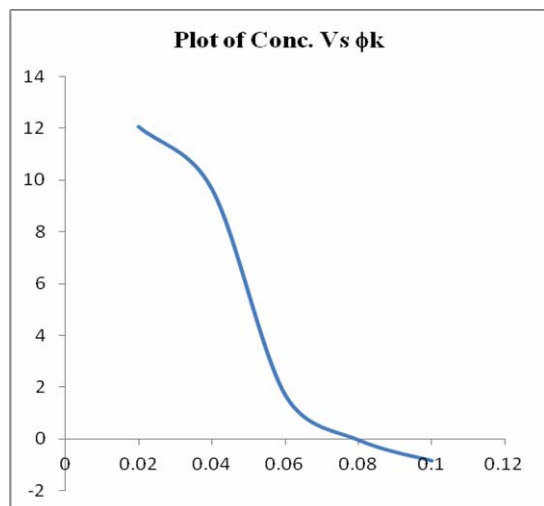


Figure 3

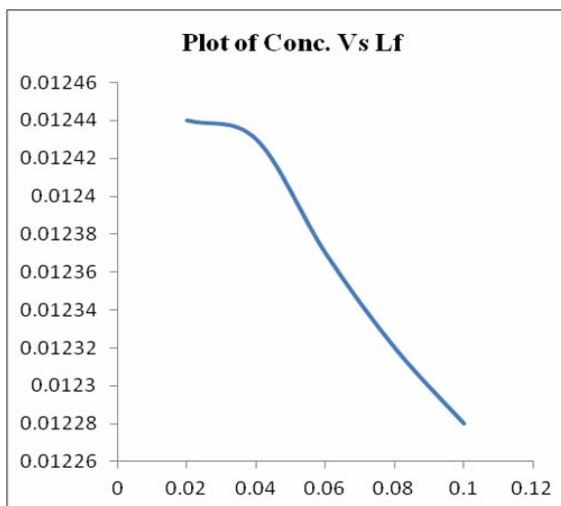


Figure 4

## References

1. S.S. Kor and S.S. Batti Indian J. Pure Appl. Phys., 1969, 7, 784.
2. S.V. Soitkar and S.N. Jajoo Acoustic Lett., 1984, 7, 191.
3. P.J. Sondawale and M.L. Narwade Ultrascience, 1999, 11(2) 162.
4. P.G. Rohankar Indian J. Chem., 2001, 40A, 860.
5. P.B. Agrawal Acta Ciencia Indica, 2003, XXIC1, 5.
6. P.B. Agrawal, Mohd. Idrees Mohd. Sidique and M.L. Narwade Indian J. Chem., 2003, 42A, 1050.
7. Ikhe, Rajput and Narwade Indian J. Chem., 2005, 44A, 2495.
8. A.B. Naik and M.L. Narwade American Erosion Journal of Scientific Research, 2008, 3(2), 229.

9. H. Gershon, R. Parmegiani and W.J. Nicerson Appl. Microbiol., 1963, 10, 556.
10. H. Gershon, R. Parmegiani Appl. Microbiol., 1963, 11, 62.
11. A.Pasynski Acta Physiochim. URSS, 8, 385, J. Phys. Chem. (USSR), 1938, 11, 608.
12. Y. Miyahava, and H.Shilo J. Chem. Soc., Japan, Pure Chem. Sect., 1952, 73, 265.
13. Y. Miyahava, and H. Shilo J. Chem. Soc., Japan, Pure Chem. Sect., 1951, 72, 876.
14. H. Asal J. Phys. Soc., Japan, 1951, 16, 761.
15. F. J. Millerio, A.L. Surdo, and C. Shin J. Phys. Chem., 1978, 82, 784.
16. S. Baluja Asian J. Chem., 2001, 13(1), 71-77.
17. B.R. Arbad, C.S. Patil, and A.G. Shankarwar Asian J. Chem., 2001, 13(1), 231-236.
18. B.R. Arbad, C.S. Patil, and A.G. Shankarwar Asian J. Chem., 2001, 13(2), 787-789.
19. S. Ubhale, N.G. Palaskar, Azhar Farooqui, R.K. Pardeshi and M.K. Lande Asian J. Chem., 2001, 13(4), 1682-1684.
20. S. Ubhale, N.G. Palaskar, Azhar Farooqui, P. M. Arif, Ali, A. S. Shankarwar Asian J. Chem., 2001, 13(4), 1685-1688.
21. P. B. Agrawal, A. S. Burghate, Mohd. Idrees and M. L. Narwade Asian J. Chem., (2001, 13(4), 1646-1648.
22. D. V. Jahagirdar, B. R. Arbad, C. S. Patil, and A. G. Shankarwar Indian J. Chem., 2001, 40A, 815-818.
23. S. D. Deosarkar<sup>1</sup> and M. L. Narwade RASAYAN J. Chem., 2010, 3(1), 55-59.
24. A. Ramtake and M. L. Narwade Arch. Appl. Sci. Res., 2012, 4(1), 254-261.
25. R. Mehra and S. Vats Int. J. of Pharma and Bio Sc., 2010, 1(4), 523-530.
26. J.H. Hildebrand "The Solubility of Non-electrolytes", Ed. 3<sup>rd</sup>, Rein Hold Publishing Corp., New York, 1950, 48.

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