Available online at www.pelagiaresearchlibrary.com

Pelagia Research Library

Pelagia Research Library

Advances in Applied Science Research, 2015, 6(9):84-88

Advances in Applied Science Research
Pelagia Research Library
ISSN: 0976-8610
CODEN (USA): AASRFC

Study of acoustical parameters of substituted aminopyrimidine by ultrasonic technique

M. M. Kalaskar, D. S. Hedaoo and M. P. Wadekar*

Applied Chemistry Division, Govt. Vidarbha Institute of Science and Humanities, Amravati, (M.S.), India

---

ABSTRACT

Ultrasonic velocity and density of substituted aminopyrimidine in 70% DMF solvent have been measured at300Kanddifferent concentration. The experimental data is used to calculate adiabatic compressibility (β_S), specific acoustic impedance (Z) and intermolecular free length (L_f). The acoustical parameters are explained on the basis of molecular interactions between the components of the mixtures. The variations of these parameters with composition of the mixture suggest the strength of molecular interactions in these mixtures.

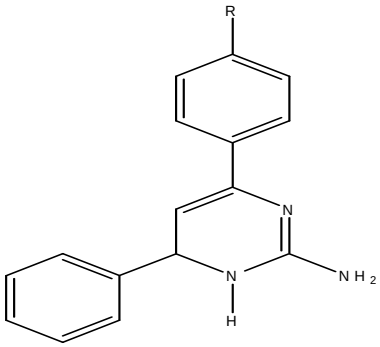
Keywords: Substituted aminopyrimidine, acoustical parameters and interactions in solutions.

INTRODUCTION

Ultrasonic study offers the most exciting and fascinating field of scientific research among the researchers since it provides useful information regarding the structure of molecules, molecular order, molecular packing, inter and intra-molecular interactions. Ultrasonic study of liquid-liquid mixture has gained much importance during the last two decades in assessing the nature of molecular interaction and investigating the physiochemical behavior of this system.

Ultrasonic technology finds a wide range of applications in medicine, biology, industry, material science, agriculture, oceanography, sonochemistry research etc. due to its non-destructive nature[1]. Ultrasonic technique is useful as a tool for phase holdup measurement in multiphase systems[2]. In field of agriculture, ultrasound waves have been utilized extensively in chemical additives (fertilizers and plant protection preparations) for improving the production yield of food produced. In materials chemistry, ultrasound waves have been useful in the preparation of biomaterials, protein microspheres, in the modification of polymers and polymer surfaces etc.[3-4]. Much work has been done in solutions of polymers [5-6], amino acids[7]and other electrolytes[8]. However, little work has been done for solutions of solid organic compounds[9-11]. Ultrasonic study of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in 70% DMF-Water is reported[12-13]. Ultrasonic study of substituted azomethine is done[14-15].Ultrasonic studies are extensively used in the conformational analysis of organic molecules. The ultrasonic study can give the indication of complex formation through hydrogen bonding in the system. Recently researchers suggested that adiabatic compressibility also used for detecting hydrogen bond formation in solutions[16].

In the present work, adiabatic compressibility (β_S), specific acoustic impedance (Z) and intermolecular free length (L_f)have been evaluated in following substituted aminopyrimidine in 70% (DMF+Water) mixture at different concentrations of ligand.



Ligand A (L_A) - *2-Amino [4-(3-nitro phenyl)-6-phenyl-1,6-dihydro]-1,3- pyrimidine*
Ligand B (L_B)- *2-Amino [4,6-diphenyl-1,6-dihydro]-1,3- pyrimidine*
Ligand C (L_C) - *2-Amino [4-(4-hydroxy phenyl)- 6-phenyl-1,6-dihydro]-1,3-pyrimidine and*
Ligand D (L_D)- *2-Amino [4-(2-hydroxy phenyl)- 6-phenyl-1,6-dihydro]-1,3-pyrimidine*

MATERIALS AND METHODS

The chemicals used were of analytical grade. Double distilled water was used for preparation of solutions. A special thermostatic water bath arrangement was made for density, ultrasonic velocity in which continuous stirring of water was carried out with the help of electric stirrer and temperature variation was maintained within $\pm 0.01^0$C. Multi frequency interferometer (Mittal Enterprises, Model MX-3) with accuracy of ±0.03% and frequency 1 MHz was used in the present work for measurement of ultrasonic velocities of solutions.

Densities of solutions were measured using specific gravity bottle of 10ml volume. These values were accurate up to ± 0.001gm. All the weighing were made on one pan digital balance (petit balance AD_50B) having an accuracy of ± 0.0001gm.

RESULTS AND DISCUSSION

The sound velocity of one ligand was measured in the concentration range of 1 x $10^{-1}$to 6.25 x 10^{-4} M in 70% DMF-Water mixture.

The distance traveled by micrometer screw get one maximum in ammeter (D), from the value of D, wavelength of ultrasonic wave is calculated using relation.

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

Where λ is wave length and D is distance in mm. The ultrasonic velocity is calculated by using relation.

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

Using the measured data some acoustical parameters have been calculated using the standard relations.
The adiabatic compressibility of solvent and solution are calculated by using equations (βs)

$$\text{Adiabatic compressibility } (\beta s) = 1/ Us^2 x\ ds \quad (3)$$

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

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

Where, U_0 and 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 (ϕ_k) of substituted aminopyrimidine in solutions are determined respectively, from density (d_s) and adiabatic compressibility(β_s) of solution using the equations

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

$\phi_k=[1000(\beta_s d_o-\beta_o d_s) / m d_s d_o] + (\beta_s M / d_s)$ (7)

where, d_o and d_s are the densities of the pure solvent and solution, respectively.

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

β_o and $\beta_s$are the adiabatic compressibilities of pure solvent and solution respectively.

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

Relative association $(R_A) = (ds /d_0) \times (U_0 /Us)^{1/3}$ (9)

Solvation number (Sn) = $\phi_k / \beta_0 x (M/ d_0)$ (10)

The value of Jacobson's constant is calculated by using relation

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

Where, T is temperature at which experiment is carried out.

Table 1: **Ultrasonic velocity, density, adiabatic compressibility (β_S), specific acoustic impedance (Z), intermolecular free length (L_f) of different concentration of substituted aminopyrimidine in 70% DMF solvent at 300K**

Conc. (m) (mol lit^{-1})	Density (ds) (kg m^{-3})	Ultrasonic Velocity(Us) (m s^{-1})	Adiabatic Compressibility (β_S) x10^{-9}(m^{2}N^{-1})	Intermolecular free length (Lf) x10^{-11}(m)	Specific acoustic impedance (Z) x10^5(kg m^{-2}s^{-1})
Ligand L_A					
0.01	1016.8	847.2	1.3702	7.6115	8.6143
0.005	1014.4	846.4	1.3760	7.6277	8.5858
0.0025	1012.8	835.2	1.4154	7.7361	8.4589
0.00125	1011.4	832.4	1.4269	7.7675	8.4188
0.000625	1010.5	805.2	1.5263	8.0334	8.1365
Ligand L_B					
0.01	1022.9	876.0	1.2739	7.3393	8.9606
0.005	1021.4	874.4	1.2805	7.3581	8.9311
0.0025	1020.9	846.4	1.3673	7.6034	8.6408
0.00125	1019.8	845.6	1.3713	7.6147	8.6234
0.000625	1017.4	823.2	1.4504	7.8311	8.3752
Ligand L_C					
0.01	1013.8	894.0	1.2341	7.2237	9.0633
0.005	1012.8	876.4	1.2855	7.3724	8.8761
0.0025	1011.9	849.6	1.3690	7.6083	8.5971
0.00125	1011.2	836.8	1.4122	7.7274	8.4617
0.000625	1010.4	813.2	1.4966	7.9548	8.2165
Ligand L_D					
0.01	1022.5	877.6	1.2698	7.3273	8.9734
0.005	1021.8	874.4	1.2800	7.3567	8.9346
0.0025	1021.1	848.0	1.3618	7.5883	8.6589
0.00125	1020.6	841.2	1.3846	7.6515	8.5852
0.000625	1019.9	836.0	1.4029	7.7017	8.5263

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

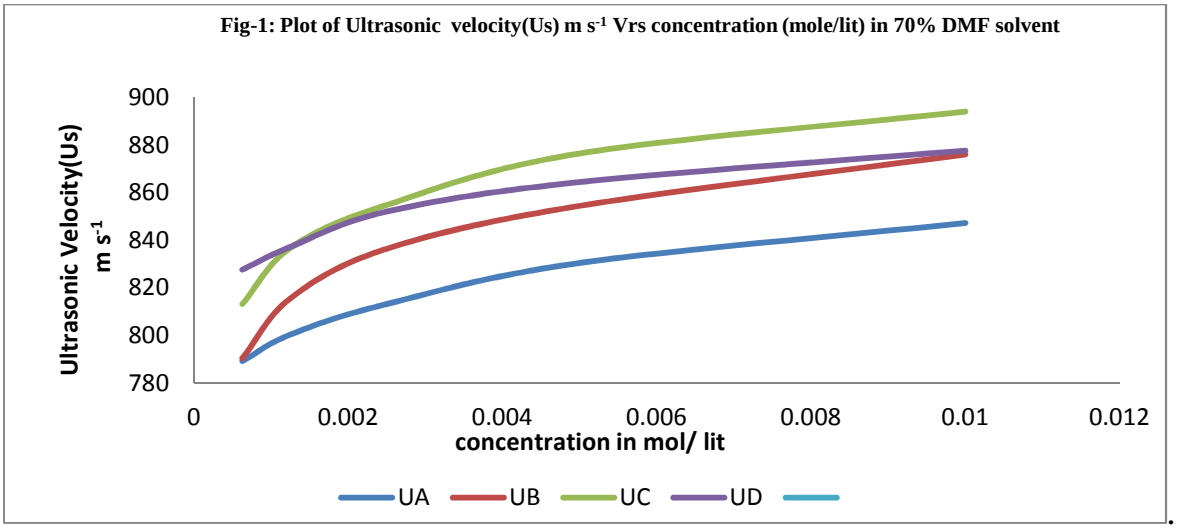


Fig-2: Plot of Adiabatic compressibility (βS) x10^{-9} m^2N^{-1} Vrs concentration (mole/lit) in 70% DMF solvent

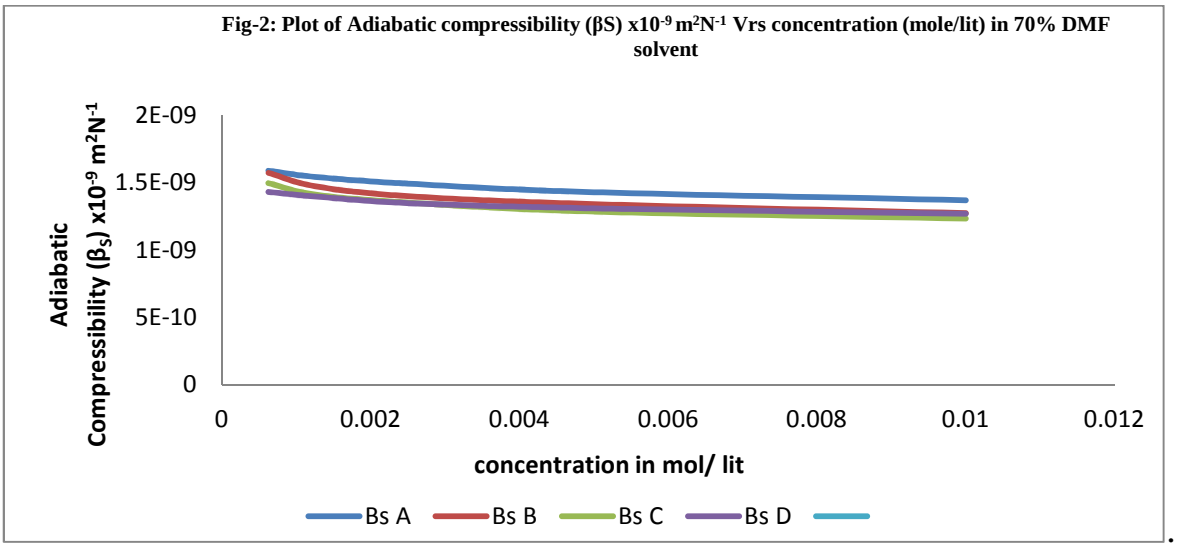
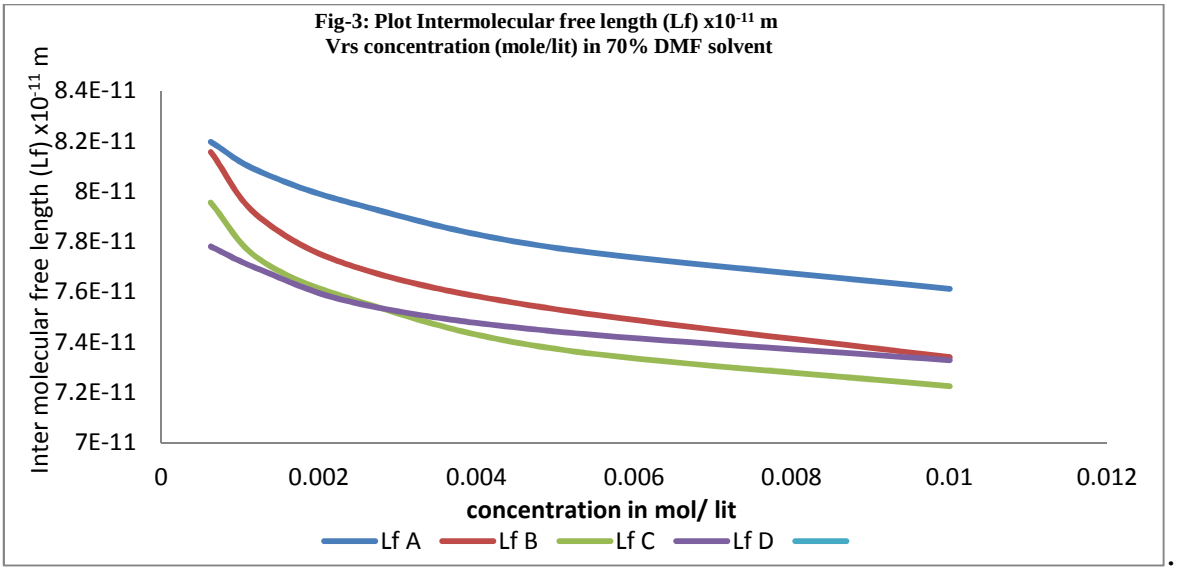
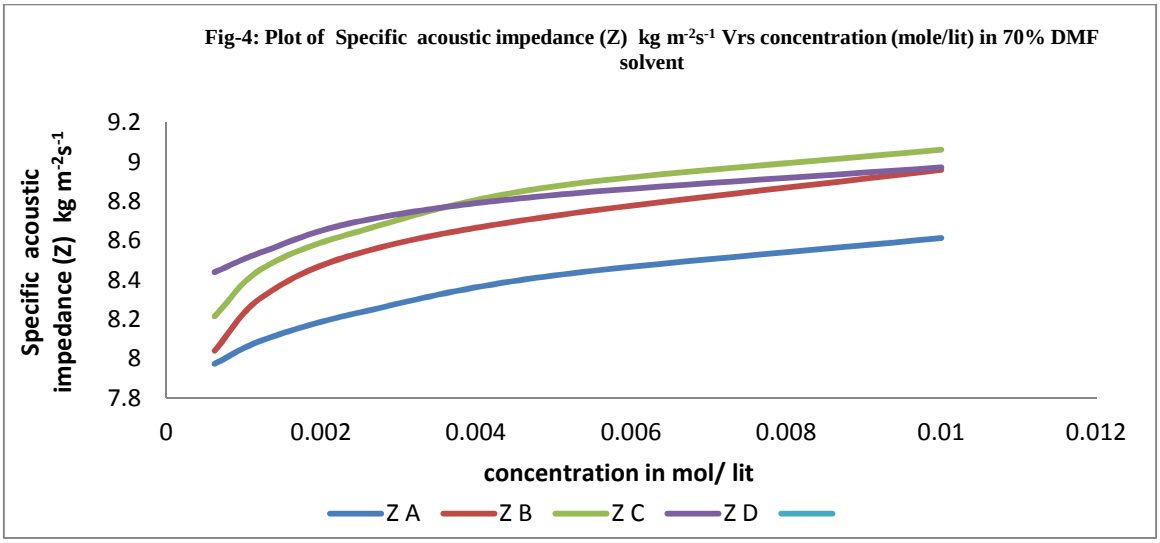


Fig-3: Plot Intermolecular free length (Lf) x10^{-11} m Vrs concentration (mole/lit) in 70% DMF solvent





From table no. 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 aminopyrimidine 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 aminopyrimidine in different solution of DMF+water mixture (fig. 3). The intermolecular free length increases 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 allsubstituted aminopyrimidine in 70% solutions of (DMF+water) mixture (fig.4).

Acknowledgement
The authors gratefully acknowledge The Director; Head, Department of Chemistry, Govt. Vidarbha Institute of Science and Humanities, Amravati for providing necessary facilities and help when needed for the work.

REFERENCES

[1] O. Kruger, T. L. Schulze, D. Peters,*Ultra. Sonochem.*,**1999**,6,123.
[2] M. Vatanakul, Y. Zheng, Couturier M, *Ind. Eng. Chem. Res.*, **2004**, 43, 5681.
[3] L. Palmowski, L. Simons, R. Brooks, *Water Sci. Tech.*, **2006**, 53(8), 281.
[4] K. S. Suslick, *Rev. Mater. Sci.*, **1999**, 29, 295.
[5] A. Ali, A. K. Nain, V. K. Sharma, S. Ahmad, *Ultrasonic Phy. Chem. Liq.*, **2004**,42, 375.
[6] V. Kannappan, S. Mahendran, P. Sathyamoorthy, D. Roopsingh, *J. Poly. Mat.*, **2001**,18, 16.
[7] R. Gomes ,M. J. Andrade ,M. Santos, S. Lima ,R. A. Gouveia ,M. M. Ferreira J. Aniceto, *Cardio. Ultra.*,**2009**,7,36.
[8]E. S. Balankina, A. K. Lyashchenko, *J. Mol. Liq.*, **2002**,101, 273.
[9] M. Mecozzi, M. Amici, E. Pietrantonio, G. Romanelli, *Ultra. Sonochem.*,**2002**,9,11.
[10] C. C. Deshmukh, A. G. Doshi, P.Agrawal,*ActaCien.Indi*,**2003**,29, 5.
[11] S. Baluja, S. Oza, *Fluid Phase Equilib.*,**2003**,208, 83.
[12] D. S. Hedaoo, M. M. Kalaskar, M. P. Wadekar, *Der PharmaChemica*, **2015**, 7(6), 245.
[13] D. S. Hedaoo, M. M. Kalaskar , M. P. Wadekar, *Adv. Appl. Sci. Res.*, **2015**, 6(6), 81.
[14] A. V. Kawalkar, D. S. Hedaoo, M. P. Wadekar, *J. Chem. Pharm. Res.*, **2015**, 7(8), 592.
[15]A. V. Kawalkar, M. P. Wadekar, *Der PharmaChemica*, **2015**, 7(8), 170.
[16] R.Sharma, Ph.D. Thesis, C.S.J.M. University, Kanpur, India,**2002**.