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Ultrasonic study of substituted aminopyrimidine in 70% DMF-water mixture

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ABSTRACT

From the experimental data, the acoustical parameters apparent molal volume (ϕ_v), apparent molalcompressibility (ϕ_κ), relative association (R_A) and solvation number (Sn) have been computed and presented as functions of compositions. 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 molecular interactions in these mixtures.

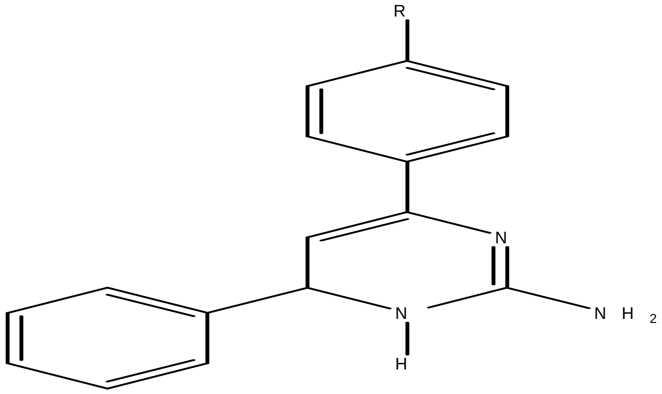
Keywords: Substituted aminopyrimidine, acoustical parameters and interactions in solutions.

INTRODUCTION

In the recent years, 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 physicochemical studies. 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[1-2]. Number of workers have made ultrasonic study of electrolytic solutions and discussed about the variation of ultrasonic velocity with ion concentration[3-7]. The understanding of the physicochemical behavior of binary and multicomponent liquid mixtures is possible by investigating their acoustic properties[8]. Acoustic properties have been the subject of extensive research activity to study the intermolecular interactions in ion-solvent systems[9]. The effect of temperature on acoustical parameters and molecular interactions in liquid mixtures and salt solutions has been studied by many workers[10-11]. But compressibilities and apparent molal volumes of substituted amiopyrimidins in DMF have not been studied so far.
Most of the ultrasonic workin non-aqueous systems possesses an interpretation of solute-solvent interactions[12]. Harish Kumar and Deepika[13],Tadkalkar[14]have studied molecular velocity and molecular compressibility from ultrasonic data. Ultrasonic study of substituted azomethine is done[15-16].Pankati etal[17]haveinvestigated the adiabatic compressibility and hydration numbers of amino acids in water solvent and water-dioxane mixtures.Ultrasonic study of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in 70% DMF-Water is reported[18-19].Ikhe[20]have studied the adiabatic compressibility and apparent molal volume of some antibiotic drugs.Praharaj and Dondge[21-22]have studied the apparent molal volumes of alcohols in aqueous solutions at different temperatures.

The present attempt is made to study the other acoustical parameters such as apparent molal volume (ϕ_v), apparent molal compressibility (ϕ_κ), relative association (R_A), solvation number (Sn) of substituted aminopyrimidine in 70% of (DMF+water) mixture at different concentrations of ligand. The different substituted aminopyrimidineligand used for present work are:



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 was 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 $1 \times 10^{-1}$to 6.25×10^{-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.

$2D = \lambda$ (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)

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)

Adiabatic compressibility $(\beta s) = 1/ Us^2 x\ ds$ (3)
Adiabatic compressibility $(\beta_0) = 1/ U_0{}^2 x\ d_0$ (4)
Acoustic impedance $(Z) = Us \times ds$ (5)

Where U_0, Us are ultrasonic velocity in solvent and solution respectttively. 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
$\phi_v = (M/d_s) + [(d_o-d_s)\ 10^3] / md_sd_o$(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) = $(ds /d_0) x (U_0 /Us)^{1/3}$ (9)
Solvation number (Sn) = $\phi_\kappa / \beta_0 x (M/ d_0)$ (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: Concentration (m), relative association (R_A), apparent molal compressibility (ϕ_κ), apparent molalvolume (ϕ_v), solvation number (Sn) at 70% (DMF+ water) solvent at 300K

Conc. (m) (mollit^{-1})	Apparent molal volume (ϕ_v) (m^{3}mol^{-1})	Apparent molal compressibility (ϕ_k)x10^{-10}(m^{2}N^{-1})	Relative association (R_A)	Solvation number (Sn)
Ligand L_A				
0.01	1.4287	4.1292	1.0099	0.7487
0.005	2.7297	4.3110	1.0143	0.7817
0.0025	5.2878	4.5054	1.0197	0.8169
0.00125	10.2736	4.6593	1.0237	0.8448
0.000625	20.1571	4.7987	1.0276	0.8701
Ligand L_B				
0.01	1.3442	3.2382	1.0047	0.6937
0.005	2.6227	3.4130	1.0116	0.7312
0.0025	5.2014	3.5666	1.0183	0.7641
0.00125	10.2086	3.7590	1.0258	0.8053
0.000625	19.5632	4.0172	1.0341	0.8606
Ligand L_C				
0.01	1.2153	3.3407	0.9890	0.6723
0.005	2.3822	3.4826	0.9946	0.7008
0.0025	4.6771	3.6679	1.0020	0.7381
0.00125	9.2178	3.8332	1.0085	0.7714
0.000625	18.1229	4.0665	1.0173	0.8183
Ligand L_D				
0.01	1.4216	3.4389	1.0037	0.6920
0.005	2.8106	3.5494	1.0081	0.7143
0.0025	5.5557	3.6581	1.0123	0.7362
0.00125	11.0177	3.7931	1.0177	0.7633
0.000625	21.7721	3.8860	1.0209	0.7820

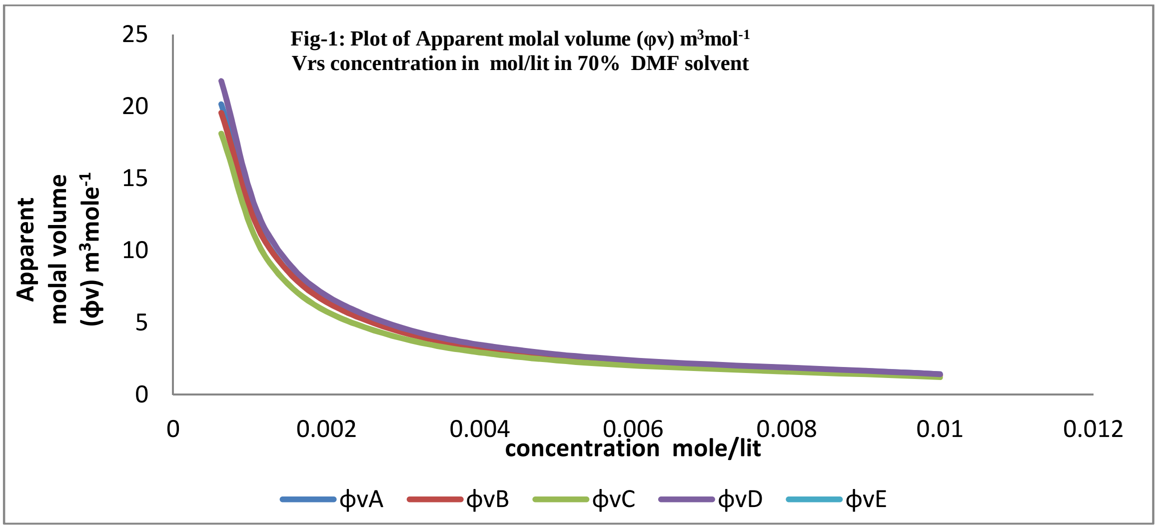


Fig-2: Plot of Apparent molal compressibility (φk) x10^{-10} m^2N^{-1} Vrs concentration in mole/lit in 70% DMF solvent.

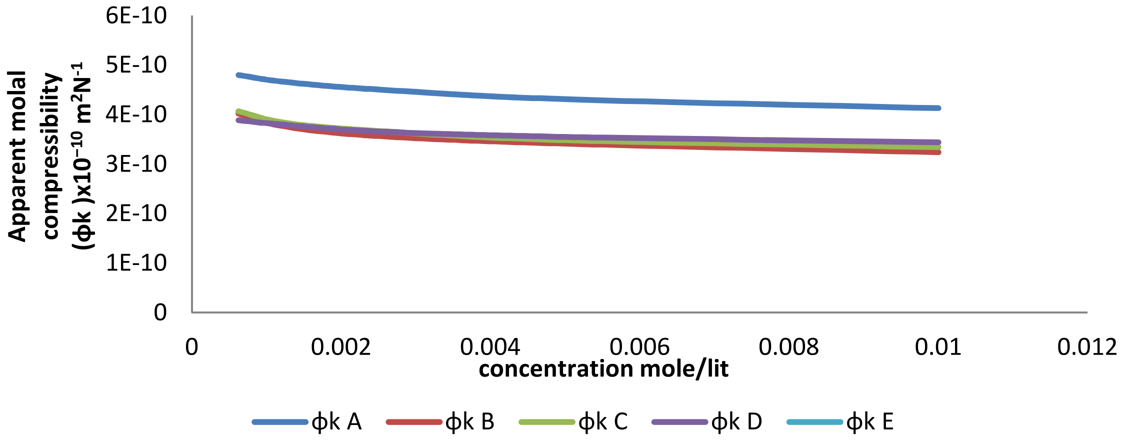


Fig-3: Plot of Relative association (RA) Vrs concentration in mole/lit in 70% DMF solvent.

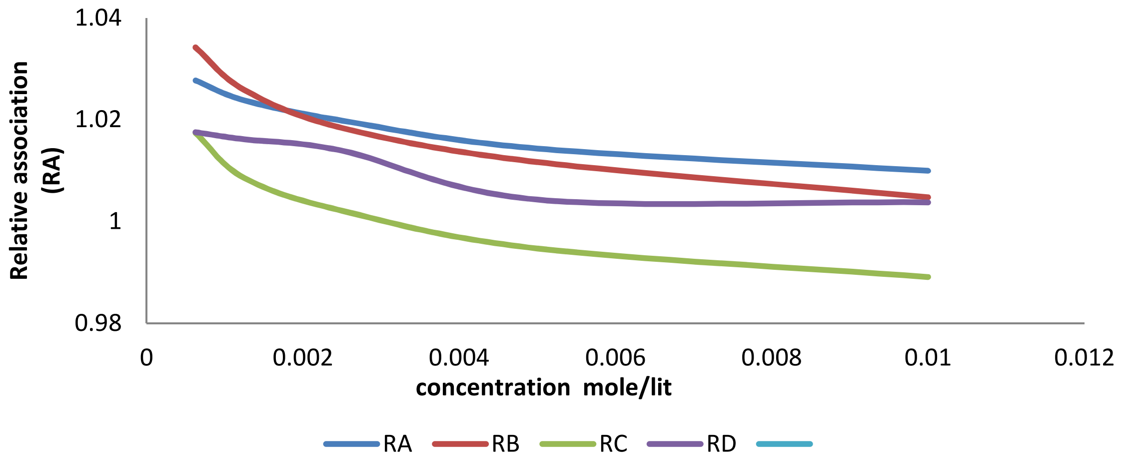
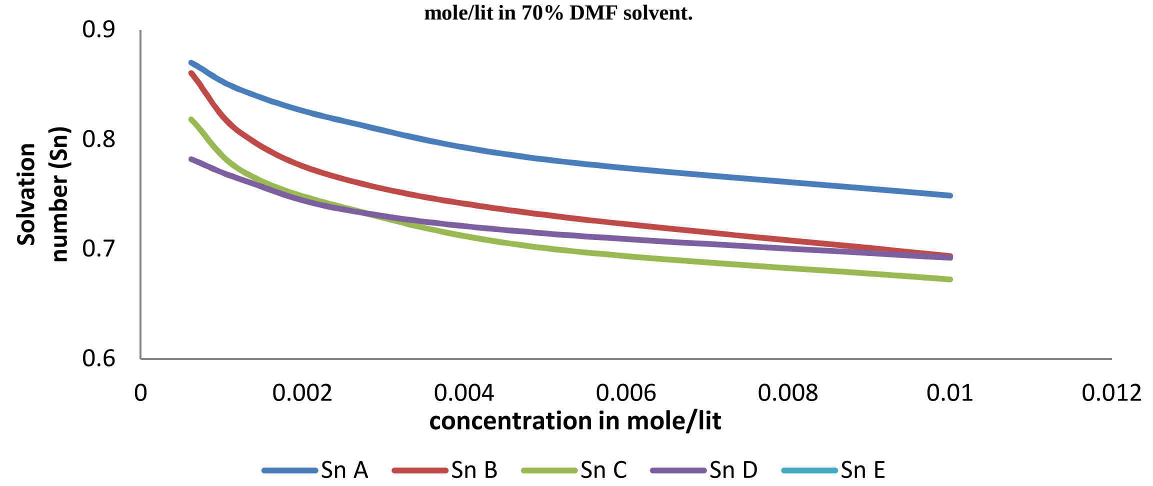


Fig-4: Plot of Solvation number (Sn) Vrs concentration in mole/lit in 70% DMF solvent.



From table no. 1, it is observed that apparent molal volume increases with decrease in concentration in all systems indicates the existence of stronge ion-solvent interaction(fig.1). The value of apparent molal volume is high in case of more polar substituent than less polar substituents. The value of apparent molal compressibility increases with decrease in concentration of all systems in 70% of (DMF+water) mixture (fig.2), showing weak electrostaticattractive force in the vicinity of ions causing electrostatic salvation of ions. Compressibility is more in case of bulky substituents. The value of relative association increases with decrease in concentration in all systems (fig.3). It is found that there is weak interaction between solute and solvent. Relative association is more in case of bulky and more polar substituents. The solvation number increase with decrease in concentration due to weak solute-solvent interaction (fig.4). The solvation number in all system increases with decrease in concentration solute indicates the large solvent molecule are present around the solute molecule which increase the solubility of solute.

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