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Adiabatic compressibility, apparent molal volume, apparent molal compressibility and solvation number of 2,3-Dihydroquinazolin-4(1*H*)-one derivatives in 70% DMF-Water

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ABSTRACT

Density and ultrasonic velocity measurements are carried out for substituted -2,3-dihydroquinazolin-4(1H)-ones in 70% DMF-Water at T= 303K. The experimental values are used to calculate adiabatic compressibility, apparent molal volume, apparent molal compressibility and solvation number. These acoustical parameters obtained are used to explain the interaction taking place in the solutions.

Keywords: Substituted-2,3-dihydroquinazolin-4(1H)-ones, acoustical parameters and interactions in solutions.

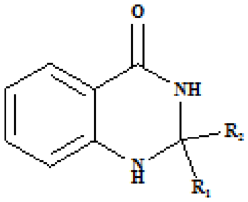
INTRODUCTION

The ultrasonic measurements are useful to determine number of acoustical parameters. The apparent molal volume has proved to be a simple and convenient tool for studying solute-solvent interactions in solutions[1]. The apparent molal volumes and compressibilities of aqueous solutions of some transition metal chlorides in the molality range $0.0 \leq m \leq 1.0$ have been determined from precise density and sound speed measurements at 25^0C[2]. Ultrasonic velocities of solutions of monochloroacetic acid in aqueous ethanol are measured by using single crystal interferometer. The ultrasonic velocity, density and concentrations are used to calculate adiabatic compressibility, intermolecular free length and apparent molal compressibility[3]. Ultrasonic velocity, density and adiabatic compressibility for 2,6-dimethylpyridine + water are measured over the entire composition range in the temperature range 293-318K[4]. The partial molal volumes and partial molal compressibilities of solutes in water and aqueous solutions are considered important thermodynamic quantities, whose knowledge hopefully gives information about the structural influence of the solute upon water structure[5].

The ultrasonic measurement shows that ultrasonic velocity, apparent molar compressibility and apparent molar volume of the solution of manganese soaps increase while adiabatic compressibility and solvation number decreases with increasing concentration of soaps. It indicates that there is significant interaction between the soap and solvent molecules in dilute solutions[6]. Compressibility is known as an independent and effective tool for investigating biologically active compounds and finds increasing use as a means for characterizing protein systems[7]. Ultrasonic velocity and adiabatic compressibility have been determined at 298.16 K for some fluorocarbon liquid mixtures over entire composition range[8]. Ultrasound velocity measurements carried out in solutions allow the determination of the compressibility of a fluid in relation to inter- and intramolecular interactions which can be characterized by the variation of thermodynamic parameters such as temperature, pressure and volume[9]. Sound velocity measurement is a widely used method for determining the compressibility of liquids, solutions, solutes and macromolecules and for the determination of a wide range of thermodynamic parameters[10]. The study of apparent molal volume and adiabatic compressibility is reported by many workers[11-15].

2,3-Dihydroquinazolin-4(1*H*)-one derivatives are playing crucial role in the context of drug intermediates, biological and pharmaceutical applications[16-20]. They have drawn much more attention because of their activities such as antibacterial[21], diuretic[22], anticancer[23], antihyperlipidemic[24], antiparkinsonism[25], antimicrobial[26], anti-inflammatory[27], bronchodilator[28], antihypertensive[29], antiproliferative[30] and antimitotic[31] activities. The data on some of the properties associated with the liquids and liquid mixtures like density, viscosity, refractive index, surface tension, and ultrasonic velocities find extensive application in solution theory and molecular dynamics[32]. These modern days there is an upsurge in topical formulations such that it can be prepared by varying physico-chemical properties and providing better localized action[33].

Ultrasonic study of number of compounds is done by many workers[34-38]. A survey of the literature indicates that no acoustical data on substituted-2,3-dihydroquinazolin-4(1*H*)-ones has been produced. In the present work, different properties such as adiabatic compressibility (β_s), apparent molal volume (ϕ_v), apparent molal compressibility (ϕ_k) and Solvation number (Sn) have been evaluated in following substituted-2,3-dihydroquinazolin-4(1*H*)-ones in 70% (DMF+Water) mixture at different concentrations of ligand.



L_A : R_1 = 4-hydroxy-3-methoxyphenyl
L_B : R_1 = 2-hydroxyphenyl
L_C : R_1 = 3-hydroxyphenyl
L_D : R_1 = 4-hydroxyphenyl
R_2 = H for all

Ligand A (L_A)= *2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one*
Ligand B (L_B)= *2-(2-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*
Ligand C (L_C)= *2-(3-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*
Ligand D (L_D)= *2-(4-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*

MATERIALS AND METHODS

The ligands of which physical parameters are to be explored are synthesized by using reported protocol[39]. All the chemicals used are of analytical grade. The density measurements are made with the precalibrated bicapillary pyknometer. All the weighings are made on one pan digital balance (petit balance AD-50B) with an accuracy of $\pm$ 0.001 gm. The speed of sound waves is obtained by using variable path crystal interferrometer (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 is employed. The instrument is calibrated by measuring ultrasonic velocity of water at 25^{o}C.

RESULTS AND DISCUSSION

Sound speeds can be measured using a single frequency ultrasonic interferometer. The ultrasonic waves of known frequency produced by a quartz crystal are reflected by a movable metallic plate kept parallel to the quartz plate. When the state of acoustic resonance is reached due to the formation of standing waves, an electrical reaction occurs on the generator driving the quartz plate and its anode current becomes maximum. The micrometer is slowly moved until the anode current meter on a high frequency generator shows a maximum. The distance thus moved by the micrometer gives the values of wavelength[40].

The distance traveled by micrometer screw to get one maximum in ammeter (D) is used to calculate wavelength of ultrasonic wave using following relation:

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

Where, λ is wavelength and D is distance in mm.

From the knowledge of the wavelength, the ultrasonic velocity can be obtained by the relation:

Ultrasonic velocity (U) = λ x Frequency x 10^3 (2)

Using the measured data some acoustical parameters can be calculated using the standard relations.

The adiabatic compressibility[41-42] of solvent and solution can be calculated by using equations:

Adiabatic compressibility of solution (βs) = $1/ Us^2$ x ds (3)

Adiabatic compressibility of solvent (β_0) = $1/ U_0^2$ x d_0 (4)

The acoustic impedance (Z) [43-44] is calculated using equation:

Acoustic impedance (Z) = Us x ds (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 compressibility (ϕ_k) are given by following equations[45-46].

Apparent molal volume $(\phi_v) = \frac{M}{d_s} + \frac{(d_o - d_s)\times 10^3}{(m d_s d_0)}$ (6)

Apparent molal compressibility $(\phi_k) = \frac{1000(\beta_s d_o - \beta_o d_s)}{m d_s d_o} + \frac{\beta_s M}{d_s}$ (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 β_s are the adiabatic compressibility of pure solvent and solution respectively.

According to the studies intermolecular free length (L_f) [47] is given by:

Intermolecular free length (L_f) = K√βs (8)

The constant K is called the Jacobson's constant.

The value of Jacobson's constant can be calculated by using relation

K = (93.875 + 0.375 x T) x 10^{-8} (9)

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

The relative association (R_A) [48-49] is given by the equation:

Relative association $(R_A) = \left(\frac{d_s}{d_o}\right) \times \left(\frac{U_o}{U_s}\right)^{1/3}$ (10)

The solvation number (S_n) [50] is given by the equation.

Solvation number (Sn) = ϕ_k /β_0 x (M/ d_0) (11)

In the present work the measurements of ultrasonic velocity and density at different concentration of substituted 2,3-dihydroquinazolin-4(1*H*)-ones in 70 % DMF-Water are carried out at *T*= 303K. The data obtained is used to evaluate different acoustical parameters such as adiabatic compressibility (β_s), apparent molal volume (ϕ_v), apparent molal compressibility (ϕ_k) and solvation number (Sn). The formula No. 03, 06, 07 and 11 are used to do calculations for acoustical parameters.

Acoustic parameters are helpful to understand behavior of solute and solvent molecules in solutions. Changes in the values of these parameters with concentration are very important to explain number of factors.

The measurement of ultrasonic velocity in pure liquids and mixtures is an important tool to study the physic-chemical properties and also explains the nature of molecular interactions. From the table no. 01, ultrasonic velocity is directly proportional to the concentration. Fig. no. 01 shows the variation of ultrasonic velocity with concentration. In more concentrated solution the possibility of making hydrogen bond increases which gives packed structure and accordingly ultrasonic velocity increases. Ultrasonic velocity increases on increasing the concentration of solute may be attributed to cohesion brought about by the association among the molecule and greater solute - solvent interaction.

Compressibility gives the ease with which a medium can be compressed. Table no. 01 shows that the adiabatic compressibility (β_s) increases with decrease in the value of concentrations. Fig. no.02 shows the variation of adiabatic compressibility with concentrations. This is as per general trend observed for the electrolytic solutions. In more concentrated solution, more cohesion is expected and this lead to a decrease in β_s. The decrease in β_s results in an increase in the value of ultrasonic velocity. 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. Adiabatic compressibility is more in case of bulky and less polar substituents. The adiabatic compressibility value decreases with increasing concentration indicates formation of strong hydrogen bonding between solute and solvent.

The concentration dependence of the apparent molal volume (ϕ_v) is very useful tool in elucidating ion-ion interactions. Table no. 01 suggests that as the concentration decreases apparent molal volume increases. Fig. no. 03 shows the variation of apparent molal volume with concentrations. The increase in apparent molal volume with decrease in concentration indicates the existence of strong ion-solvent interaction. The value of apparent molal volume is high in case of more polar substituent than less polar substituents. Apparent molal volume is affected by the phenomenon of salvation. The molal concentrations dependence of apparent molal volume is useful in understanding solute-solvent interactions.

Table no. 01, suggests that apparent molal compressibility (ϕ_k) increases with decreases in concentrations. Fig. no. 04 shows the variation of apparent molal compressibility with concentrations. The increase in value of apparent molal compressibility (ϕ_k) with decrease in concentrations shows the weak electrostatic attractive force in the vicinity of ions causing electrostatic salvation of ions. Compressibility is more in case of bulky substituent.

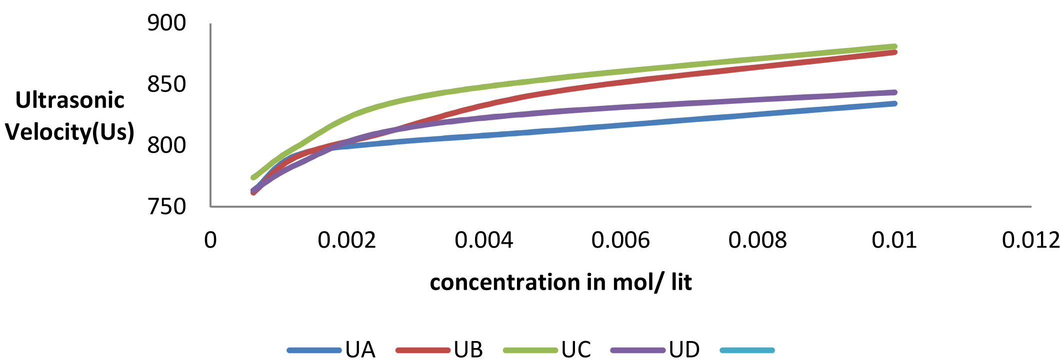
The solvation number (Sn) increases as the concentration decrease as per Table no 01. Fig. no. 05 shows the variation of solvation number with concentrations. When salvation occurs, the solvent molecules of the ion-solvent complex may be assumed to more closely packed than in the pure solvent. The solvation number increase with decrease in concentration due to weak solute-solvent interaction.

Table 1: Ultrasonic velocity, density, adiabatic compressibility (β_S), apparent molal volume (ϕ_v), apparent molal compressibility (ϕ_k), solvation number (Sn) at different concentration of substituted -2,3-Dihydroquinazolin-4(1*H*)-ones in 70% DMF solvent at 303K

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})	Apparent molal volume (ϕ_v) (m^{3}mol^{-1})	Apparent molal Compressibility (ϕ_k) x10^{-10} (m^{2}N^{-1})	Solvation number (Sn)
Ligand L_A						
0.01	1019.7	906.8	1.1926	1.2327	2.9358	0.6499
0.005	1017.7	870.8	1.2958	2.3794	3.1980	0.7079
0.0025	1015.6	835.2	1.4115	4.5767	3.4890	0.7723
0.00125	1014.2	795.2	1.5592	8.9088	3.8625	0.8550
0.000625	1011.4	771.6	1.6607	16.8306	4.1111	0.9101
Ligand L_B						
0.01	1016.4	848.4	1.3668	1.1615	3.3447	0.7404
0.005	1013.5	816.4	1.4803	2.1964	3.6239	0.8022
0.0025	1011.6	814.8	1.4889	4.2253	3.6404	0.8058
0.00125	1009.8	806.0	1.5243	8.1307	3.7262	0.8249
0.000625	1008.0	802.8	1.5393	15.6169	3.7658	0.8336
Ligand L_C						
0.01	1012.0	881.2	1.2725	1.0651	3.4959	0.7739
0.005	1011.2	854.8	1.3534	2.0949	3.5516	0.7862
0.0025	1010.6	832.8	1.4267	4.1366	3.6152	0.8003
0.00125	1006.5	798.8	1.5570	7.5380	3.7097	0.8212
0.000625	1003.7	774.0	1.6630	14.0577	3.8591	0.8543
Ligand L_D						
0.01	1008.3	843.6	1.3936	1.1097	3.9569	0.7757
0.005	1006.0	827.6	1.4513	2.1023	4.0306	0.7902
0.0025	1005.0	810.8	1.5135	4.1022	4.0817	0.8002
0.00125	1002.5	784.4	1.6212	7.6883	4.1874	0.8209
0.000625	0998.3	763.6	1.7179	13.6186	4.2245	0.8282

Graphical Representation of acoustic parameters in 70% DMF-water solvent

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



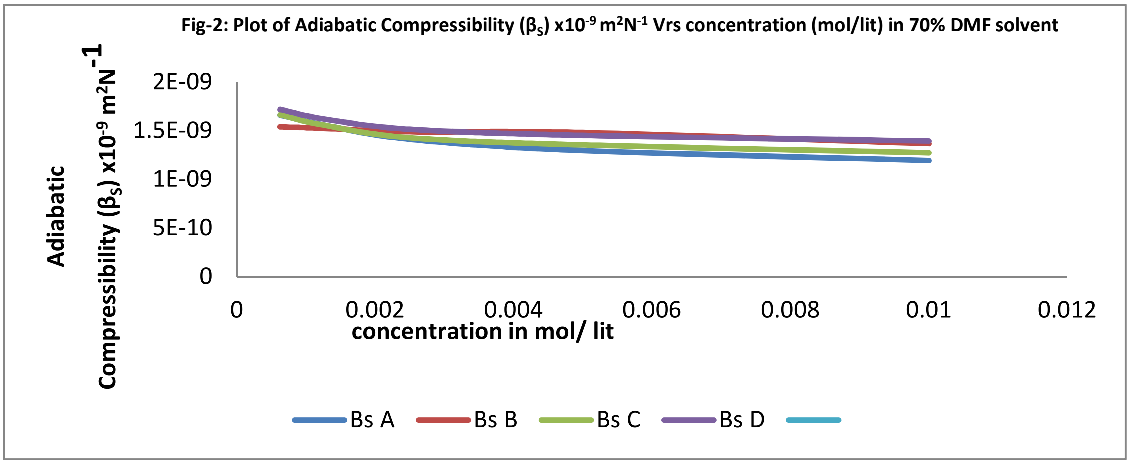


Fig-2: Plot of Adiabatic Compressibility (β_s) x10^{-9} m^2N^{-1} Vrs concentration (mol/lit) in 70% DMF solvent

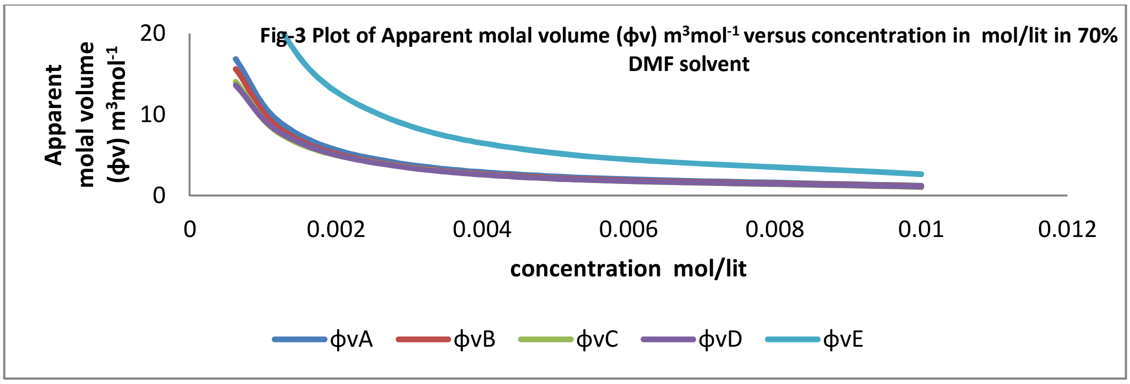


Fig-3 Plot of Apparent molal volume (ϕv) m^3mol^{-1} versus concentration in mol/lit in 70% DMF solvent

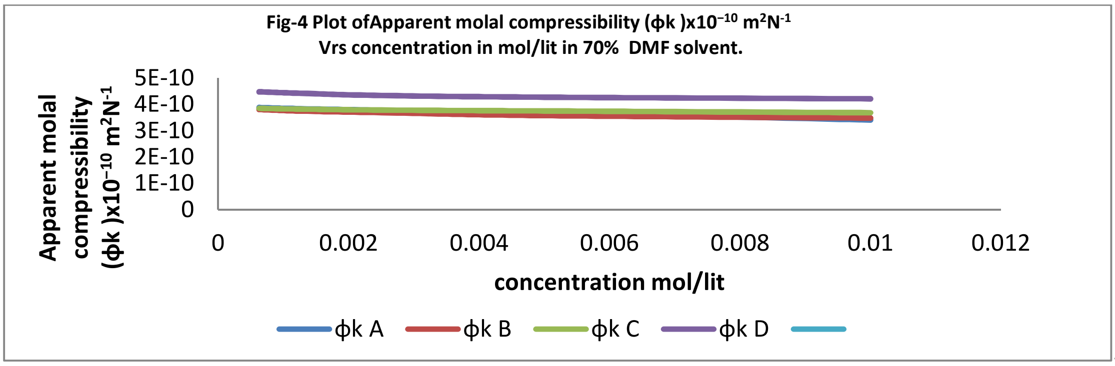


Fig-4 Plot ofApparent molal compressibility (ϕk)x10^{-10} m^2N^{-1} Vrs concentration in mol/lit in 70% DMF solvent.

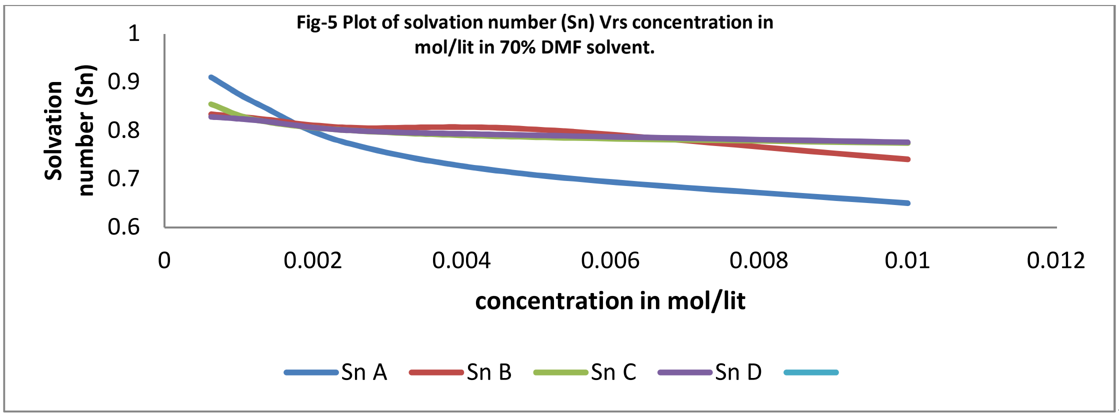


Fig-5 Plot of solvation number (Sn) Vrs concentration in mol/lit in 70% DMF solvent.

CONCLUSION

Acoustic parameters are helpful to understand behavior of solute and solvent molecules in solutions. Changes in the values of these parameters with concentration are very important to explain number of factors. In more concentrated solution the possibility of making hydrogen bond increases which gives packed structure and accordingly ultrasonic velocity increases. The adiabatic compressibility value decreases with increasing concentration indicates formation of strong hydrogen bonding between solute and solvent. The increase in apparent molal volume with decrease in concentration indicates the existence of strong ion-solvent interaction. The increase in value of apparent molal compressibility (ϕ_k) with decrease in concentrations shows the weak electrostatic attractive force in the vicinity of ions causing electrostatic salvation of ions.

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