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Ultrasonic study of substituted-2,3-dihydroquinazolin-4(1*H*)-ones 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 intermolecular free length (L_f), specific acoustic impedance (Z) and relative association (R_A). These acoustic parameters obtained are used to explain the interaction taking place in the solutions.

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

INTRODUCTION

Ultrasound is a type of energy that can help analytical chemists in almost all their laboratory tasks, from cleaning to detection[1]. Ultrasonic technique is used as a tool for phase holdup measurement in multiphase systems[2]. The effect of ultrasound on adsorption and desorption processes has been reported[3]. The structural studies of chelates by ultrasonic waves are reported[4]. The use of sound velocity to study polymer solutions is reported[5]. The study of propagation of ultrasonic waves in solution is useful for analyzing certain physical parameters. Science and technology of ultrasonic is widely used in recent years for industrial and medicinal applications[6]. The ultrasonic waves of various frequencies have found uses in areas such as medical imaging, geological imaging, industrial cleaning and welding, solution mixing and even jewelry cleaning[7]. The ultrasound finds application in microsurgery, fatigue detection in aerospace mechanics, sonochemical catalysis and biotechnology[8]. Ultrasound is used to obtain images for medical diagnostic purposes, especially during pregnancy[9]. The coagulation in milk may be prevented by intense agitation of it with ultrasonic waves[10]. Ultrasound is a powerful noninvasive modality for biomedical imaging, and holds much promise for noninvasive drug delivery enhancement and targeting[11].

The review of literature on acoustical studies of solutions reveals that ultrasonic measurements are used to estimate the different elastic properties[12]. The understanding of the physicochemical behavior of binary and multicomponent liquid mixtures is possible by investigating their acoustic properties[13]. Acoustic properties have been the subject of extensive research activity to study the intermolecular interactions in ion-solvent systems[14]. Ultrasound-promoted synthesis has attracted much attention during the past few decades[15]. 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[16].

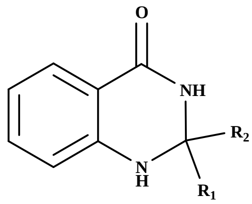
Ultrasonic velocity measurements are highly sensitive to molecular interactions and can be used to provide qualitative information about the physical nature and strength of molecular interaction in liquid mixtures[17-21]. Ultrasonic measurement in the liquid state gives information about physicochemical behavior of liquid mixtures such as molecular association and dissociation[22]. Ultrasonic study of number of compounds is done by many workers[23-27].

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

The ultrasonic measurements are used to determine number of acoustical parameters. The ultrasonic velocity, density and concentrations are used to calculate adiabatic compressibility, intermolecular free length and apparent molal compressibility[28]. Ultrasonic velocity, density and adiabatic compressibility for 2,6-dimethylpyridine + water are measured over the entire composition range in the temperature range 293-318K[29]. The study of apparent molal volume and adiabatic compressibility is reported by many workers[30-34].

2,3-Dihydroquinazolin-4(1*H*)-one derivatives are playing crucial role in the context of drug intermediates, biological and pharmaceutical applications[35-39]. They have drawn much more attention because of their activities such as antibacterial[40], diuretic[41], anticancer[42], antihyperlipidemic[43], antiparkinsonism[44], antimicrobial[45], anti-inflammatory[46], bronchodilator[47], antihypertensive[48], antiproliferative[49] and antimitotic[50] 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[51]. 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[52].

In the present work, Intermolecular free length (L_f), Acoustic impedance (Z) and Relative association (R_A) have been evaluated in following substituted 2,3-dihydroquinazolin-4(1*H*)-ones in different percentage of (DMF+Water) mixture at different concentrations of ligand.



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[53]. 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[54].

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

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

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:

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

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

The adiabatic compressibility[55-56] of solvent and solution can be calculated by using equations:

$$\text{Adiabatic compressibility of solution } (\beta s) = 1/\, Us^2 \times ds \qquad (3)$$
$$\text{Adiabatic compressibility of solvent } (\beta_0) = 1/\, U_0^2 \times d_0 \qquad (4)$$

The acoustic impedance (Z) [57-58] is calculated using equation:

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

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[59-60].

$$\text{Apparent molal volume } (\phi_v) = \frac{M}{d_s} + \frac{(d_o - d_s)\times 10^3}{(m d_s d_0)} \qquad (6)$$
$$\text{Apparent molal compressibility } (\phi_k) = \frac{1000(\beta_s d_o - \beta_o d_s)}{m d_s d_o} + \frac{\beta_s M}{d_s} \qquad (7)$$

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) [61] is given by:

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

The constant K is called the Jacobson's constant.
The value of Jacobson's constant can be calculated by using relation

$$K = (93.875 + 0.375 \times T) \times 10^{-8} \qquad (9)$$

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

The relative association (R_A) [62-63] 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) [64] 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 Intermolecular free length (L_f), Acoustic impedance (Z) and Relative association (R_A). The formula No. 05, 08 and 10 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.

Table-1: Ultrasonic velocity, density, intermolecular free length (L_f), specific acoustic impedance (Z) and relative association (R_A) at different concentration of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in 70% (DMF+Water) solvent at 303K

Conc. (m) (mol lit^{-1})	Density (ds) (kg m^{-3})	Ultrasonic velocity(Us) (m s^{-1})	Intermolecular free length (L_f) x10^{-11} (m)	Specific acoustic Impedance (Z)x10^5 (kg m^{-2}s^{-1})	Relative association (R_A)
Ligand L_A					
0.01	1019.7	906.8	7.1011	9.2466	1.0179
0.005	1017.7	870.8	7.4019	8.8621	1.0250
0.0025	1015.6	835.2	7.7254	8.4822	1.0273
0.00125	1014.2	795.2	8.1196	8.0649	1.0302
0.000625	1011.4	771.6	8.3795	7.8039	1.0401
Ligand L_B					
0.01	1016.4	848.4	7.6022	8.6231	0.9982
0.005	1013.5	816.4	7.9115	8.2742	1.0079
0.0025	1011.6	814.8	7.9345	8.2425	1.0199
0.00125	1009.8	806.0	8.0282	8.1389	1.0262
0.000625	1008.0	802.8	8.0674	8.0922	1.0373
Ligand L_C					
0.01	1012.0	881.2	7.3351	8.9177	0.9920
0.005	1011.2	854.8	7.5647	8.6437	1.0013
0.0025	1010.6	832.8	7.7668	8.4162	1.0095
0.00125	1006.5	798.8	8.1139	8.0399	1.0195
0.000625	1003.7	774.0	8.3855	7.7686	1.0274
Ligand L_D					
0.01	1008.3	843.6	7.6761	8.5060	1.0029
0.005	1006.0	827.6	7.8335	8.3256	1.0070
0.0025	1005.0	810.8	7.9998	8.1485	1.0129
0.00125	1002.5	784.4	8.2793	7.8636	1.0216
0.000625	0998.3	763.6	8.5227	7.6230	1.0265

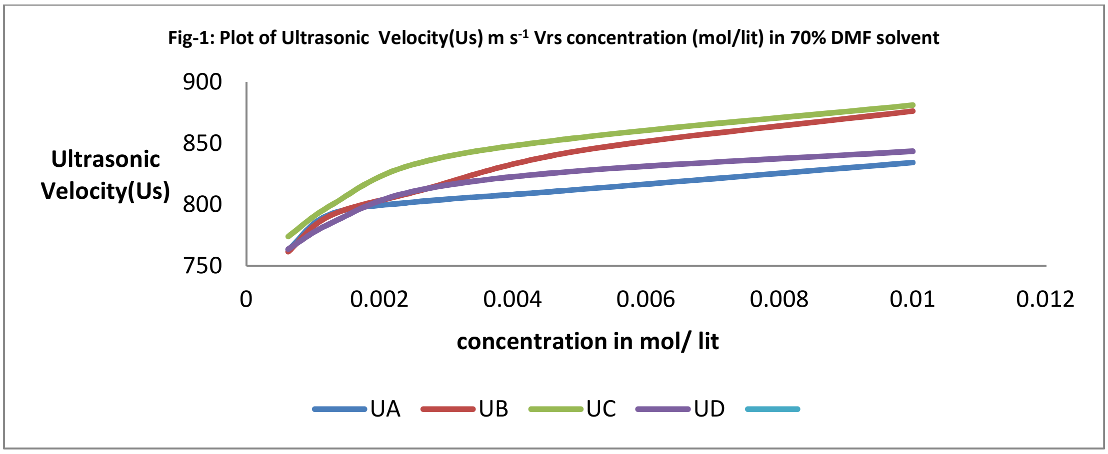
The measurement of ultrasonic velocity in pure liquids and mixtures is an important tool to study the physic-chemical properties and also explains the nature of molecular interactions. From the table no. 01, ultrasonic velocity is directly proportional to the concentration. Fig. no. 01 shows the variation 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.

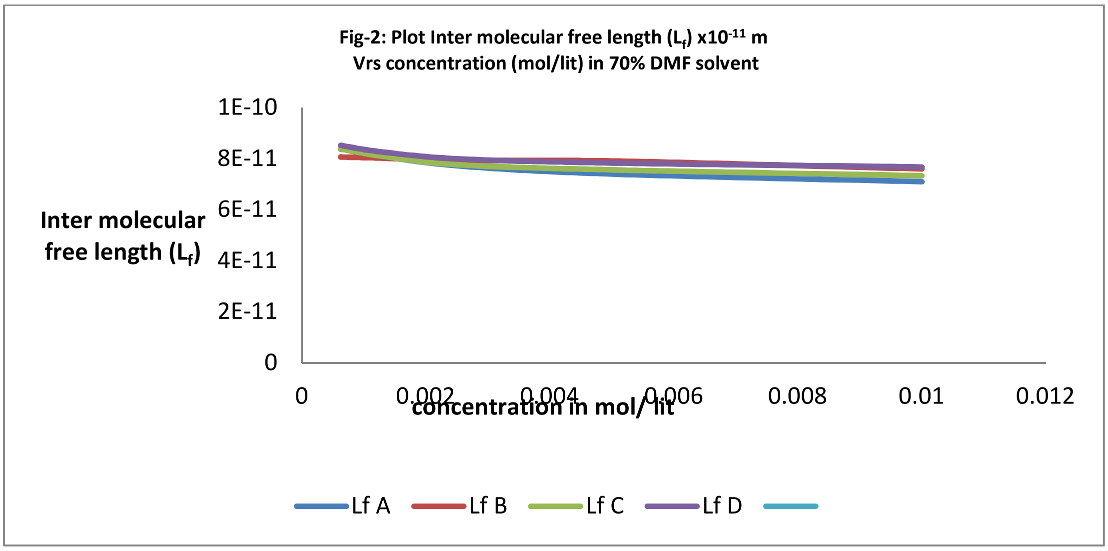
Extensive use of intermolecular free length (L_f) is made to study the intermolecular interactions in mixtures. Table no 01 suggests that intermolecular free length is more in more dilute solutions. Fig. no. 02 shows the variation of intermolecular free length with concentrations. In many cases, the value of L_f corresponds to the molecular shape, that is the L_f in the molecules having the spherical and/or symmetrical shape is short and the short L_f leads to a high speed of sound. Decrease in intermolecular free length leads to positive deviation in sound velocity and negative deviation in compressibility.

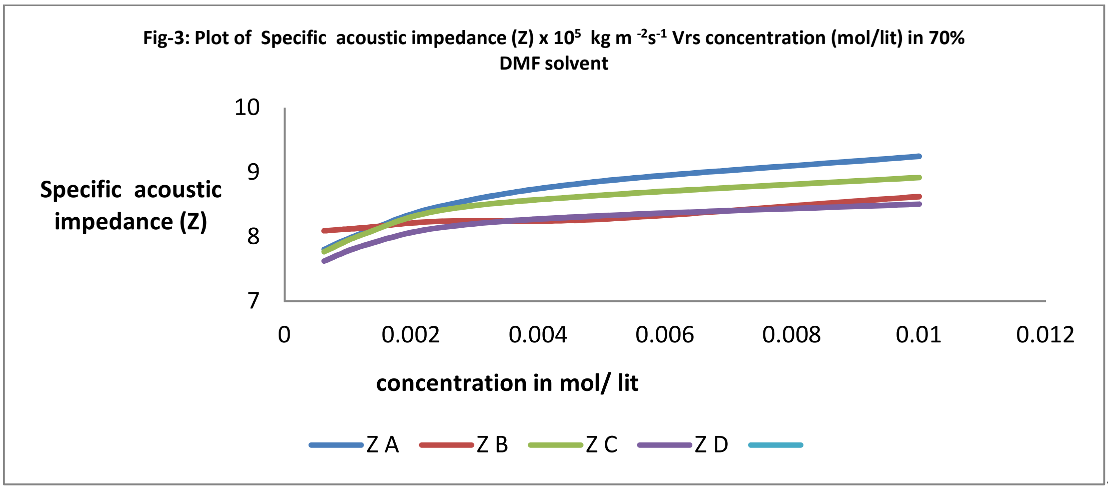
Specific acoustic impedance (Z) is the impedance offered to sound wave by the components of mixture. Table no. 01 suggests that as the concentration decreases the specific acoustic impedance decreases. Fig. no. 03 shows the variation of specific acoustic impedance with concentrations. Mathematically it is directly proportional to ultrasonic velocity. Increase in specific acoustic impedance with increase in concentration suggests associative molecular interactions.

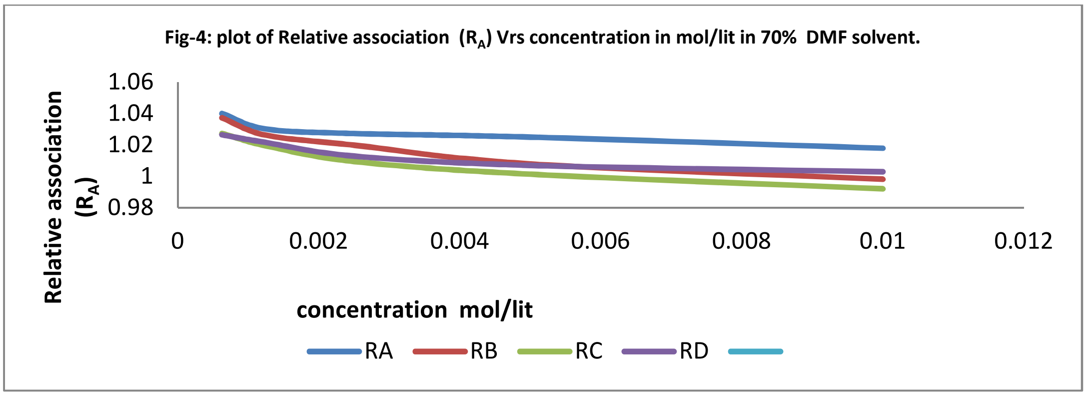
Table no. 01 shows that relative association (R_A) increases as the concentrations decreases. Fig. no. 04 shows the variation of relative association with concentrations. Relative association (R_A) is the property used to understand the solute-solvent interaction. R_A is less in case of compound having ring deactivating substituent. If compound has ring deactivating substituent then it has a less interaction with solvent molecule and hence has a greater free length.

GRAPHICAL REPRESENTATION OF ACOUSTIC PARAMETERS IN 70% DMF-WATER 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.

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