Ultrasonic and Acoustic Investigation of Aqueous Solution of Paracetamol at different pH and different temperature

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Abstract: ***Ultrasonic velocity (U) density (ρ), viscosity (η) and refractive index (n_D) have been measured at 303.15K, 308.15K, 313.15K, 318.15K and 323.15K for drug paracetamol. Various acoustical parameters such as acoustical impedance (Z), adiabatic compressibility (β) and intermolecular free length (Lf) have been calculated from ultrasonic velocity, density and viscosity data. The results have been discussed from the view point of drug solvent and intermolecular interactions.***

Index Terms - Ultrasonic velocity, Density, Paracetamol, refractive index, pH

I. INTRODUCTION

Ultrasound waves are known for their wide application in various fields [1–5] like industry, medicine, material testing, under water ranging (depth gauges, SONAR) and cleaning (ultrasonic baths). In recent years, measurements of the ultrasonic velocity have been adequately employed in understanding the nature of molecular interactions in pure liquids, liquid mixtures, and solutions [6, 7]. Drug action, although complex, results from various kinds of physicochemical interactions, e.g., ionic or covalent, charge transfer, hydrogen bonding, ion–dipole interactions, hydrophilic interactions, etc [8, 9]. Knowledge of the use of drugs involving physiological and biochemical effects, and their mechanism of action at macromolecular levels can be studied in pharmakinetics [10, 11]. The growing interest in the study of molecular interactions of drug with other biomolecules is due to the fact that these interactions are the key to understand the structural or characteristic property of drug molecules.

In this work, we have focused on the ultrasonic and acoustic investigations of paracetamol drug. Ultrasonic parameters such as ultrasonic velocity (U), density (ρ), viscosity (η), refractive index (n_D) and acoustical parameters such as adiabatic compressibility (β), intermolecular free length (L_f) and specific acoustic impedance (Z) of aqueous paracetamol solution as a function of pH and temperature were evaluated.

II. EXPERIMENTAL METHOD

Sample Preparation

1 M solution of water soluble paracetamol is obtained by adding the known numbers of molecular weight of drug Paracetamol is added into a fixed volume of solvent distilled water and stirred the solution for homogeneous solution. In the present investigation the chemicals used are of AR grade. Glass stoppered conical flasks are used for preserving the prepared mixtures and the flasks are left undisturbed to attain thermal equilibrium. Ultrasonic velocity of drug paracetamol with water over the pH range of 6.5, 7.0, 7.5, 8.0, 8.5 and have been measured at 303.15K, 308.15K, 313.15K, 318.15K and 323.15K temperature of drug was measured using a single crystal ultrasonic interferometer at 2 MHz frequency (Model M-81) supplied by Mittal enterprises, New Delhi. The density of various pH has been measured using 25 ml capacity specific gravity bottle and digital balance with an accuracy of 0.0001 gm. The viscosity at various pH has been determined by using Ostwald viscometer. Refractive indices were measured using thermostatically controlled Abbe refractometer with accuracy less than 0.0001 units. The pH of the solution was determined using ELICO (India) electronic pH meter (Model LI 120). The pH meter is standardized using low and high pH buffer tablets provided by the manufacturer.

Theory and calculations

From the experimental data of ultrasonic velocity (U), density (ρ), viscosity (η) and refractive index (n_D) various acoustic and thermodynamic parameters were calculated using following standard equations.

Adiabatic compressibility (β)

The adiabatic compressibility (β) has been calculated from the ultrasonic velocity (U) and density (ρ) of the medium using the equation as:

$$\beta = 1/U^2\rho \ (\text{kg}^{-1}\text{ms}^{-2}) \qquad \ldots\ldots\ldots\ldots\ldots (1)$$

Specific Acoustic impedance (Z)

The specific acoustic impedance is given by following equation, where U and ρ are the ultrasonic velocity and density of the liquid respectively.

$$Z = \rho U \ (\text{kg m}^{-2}\ \text{s}^{-1}) \qquad \ldots\ldots\ldots\ldots (2)$$

Intermolecular free length (L_f)

Intermolecular free length has been determined as:

$$L_f = K_T \beta^{1/2} \ (\text{m}) \qquad \ldots\ldots\ldots\ldots (3)$$

Where K is temperature dependent constant called as Jacobson constant it is 2.075×10^{-6} for 303.15K.

III. RESULTS AND DISCUSSION

The results obtained in the present study in terms of ultrasonic and acoustic parameters of drug Paracetamol in water over the pH range of 6.5, 7, 7.5, 8, and 8.5 and have been measured at 303.15 K, 308.15K, 313.15K, 318.15K and 323.15K temperature and it is represented by fig. 1-7 and tabulated in table 1-2.

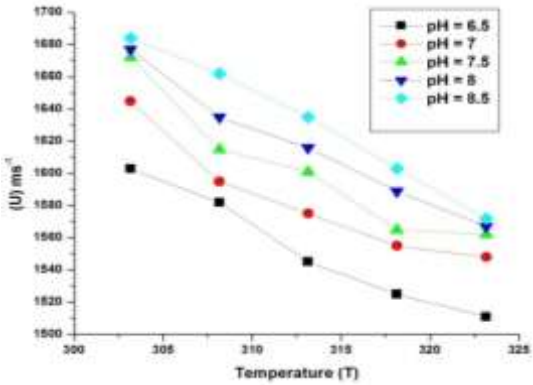

Figure 1: Variation of Ultrasonic velocity (U) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

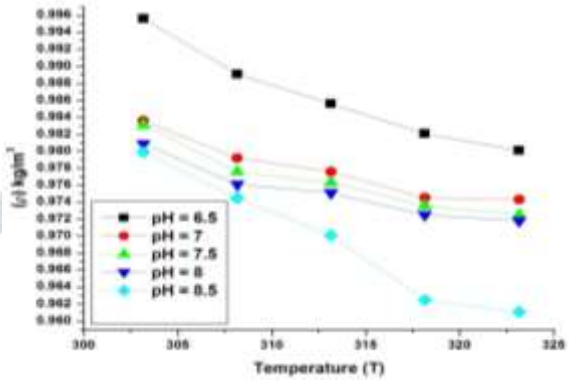

Figure 2: Variation of Density (ρ) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

The variation of ultrasonic velocity against the pH for five different temperatures and pH also represented graphically. It is observed from fig. 1 that the ultrasonic velocity was found to decrease with increasing temperature [12]. Which is clearly shows that molecular association is being takes place in the solution. Variation of ultrasonic velocity in solution depends upon the increase or decrease of molecular free length after mixing the solute (fig.1).

Intermolecular free length increases linearly on increasing the temperature of solution. This shows that there is more force of interaction between solute and solvent by forming hydrogen bonding. This was happened because there is more significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the solution. This may also specifies that increase in number of free ions showing the occurrence of ionic association due to stronger ion-ion interaction (fig. 3). The decreased compressibility brings the molecules to a closer packing resulting in a decrease of intermolecular free length with increase in drug pH [13]. Refractive Index (n_D) of water soluble paracetamol has been determined for various pH by using Abbe Refractometer at temperature 303.15 K, 308.15 K, 313.15 K, 318.15 K and 323.15 K with different pH and presented in Table 1 and graphically represented in Figure 4. It is observed from respective tables that refractive index increases with increase in pH and decreases with increase in temperature.

The specific acoustic impedance (Z) decreases with increase in temperature and increases with pH, the decreased behavior is due to the effect of weak solute-solvent interaction existing in the solutions (fig. 6). Adiabatic compressibility increases with increase in temperature may be due to gain of solvent molecule around ions, this supporting weaker ion-solvent interaction. The increase in adiabatic compressibility and decrease in ultrasonic velocity shows thereby weaker intermolecular interaction (fig. 5). The ultrasonic velocity increases whereas adiabatic compressibility decreases with increase in pH [13]. This indicates that there is strong solute solvent interaction. The solution becomes more and more compressible as value of pH increases. When pH of solution is increased in solution, ions attracted certain drug molecules towards it by moving with a violent twist in the bulk of ions due to the force of electrostriction. The rise of the temperature is accompanied by a decrease of the viscosity (fig. 3). It is observed from Table 1 and graphically represented in Figure 3 that viscosity decreases with increase in pH as well as density of the solution (fig. 2). Density of various temperatures and pH of water soluble paracetamol is listed in Table 1. It is observed from Table 1 and graphically represented in fig. 2 that that the density decreases with increase in temperature and pH of sample [14].

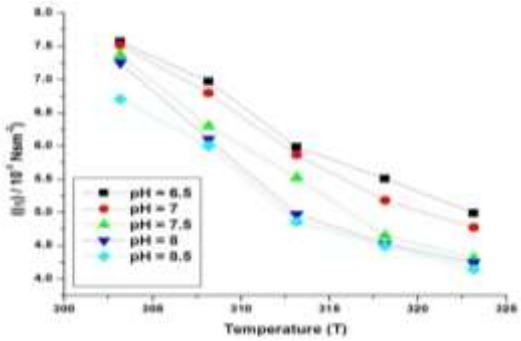

Figure 3: Variation of Viscosity (η) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

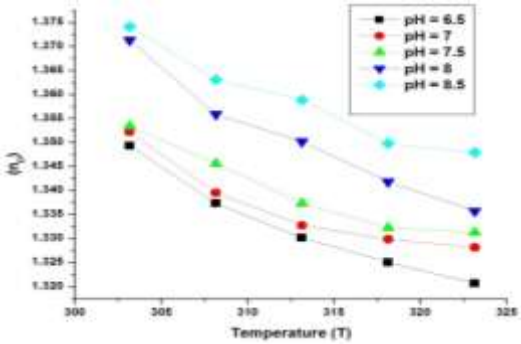

Figure 4: Variation of Refractive index (n_D) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

Table 1: Ultrasonic velocity (U), density (ρ), viscosity (η) and refractive index (n_D) for Paracetamol + Water system at pH from 6.5to 8.5 and at temperatures 303.15 to 323.15K

Concentration (M) = 0.1 M					
pH	**Temp. (K)**	**(U) ms^{-1}**	**(ρ) kg/m^3**	**(η) / 10^{-3} Nsm^{-2}**	**(n_D)**
6.5	**303.15**	**1603**	**0.9956**	**7.5692**	**1.3493**
	308.15	**1582**	**0.9891**	**6.9721**	**1.3373**
	313.15	**1545**	**0.9856**	**5.9845**	**1.3301**
	318.15	**1525**	**0.9821**	**5.5077**	**1.3250**
	323.15	**1511**	**0.9801**	**4.9878**	**1.3207**
7	**303.15**	**1645**	**0.9836**	**7.5173**	**1.3522**
	308.15	**1595**	**0.9792**	**6.7968**	**1.3395**
	313.15	**1575**	**0.9776**	**5.8644**	**1.3327**
	318.15	**1555**	**0.9745**	**5.1806**	**1.3298**
	323.15	**1548**	**0.9743**	**4.7712**	**1.3281**
7.5	**303.15**	**1672**	**0.9831**	**7.3641**	**1.3534**
	308.15	**1615**	**0.9776**	**6.3009**	**1.3456**
	313.15	**1601**	**0.9763**	**5.5217**	**1.3373**
	318.15	**1565**	**0.9736**	**4.6479**	**1.3322**
	323.15	**1562**	**0.9725**	**4.3082**	**1.3312**
8	**303.15**	**1677**	**0.9809**	**7.2572**	**1.3713**
	308.15	**1635**	**0.9761**	**6.1065**	**1.3559**
	313.15	**1616**	**0.9751**	**4.9743**	**1.3502**
	318.15	**1589**	**0.9725**	**4.5231**	**1.3418**
	323.15	**1567**	**0.9718**	**4.2381**	**1.3357**
8.5	**303.15**	**1684**	**0.9799**	**6.7063**	**1.3741**
	308.15	**1662**	**0.9745**	**6.0024**	**1.3631**
	313.15	**1635**	**0.9701**	**4.8563**	**1.3589**
	318.15	**1603**	**0.9625**	**4.4877**	**1.3498**
	323.15	**1572**	**0.9611**	**4.1475**	**1.3479**

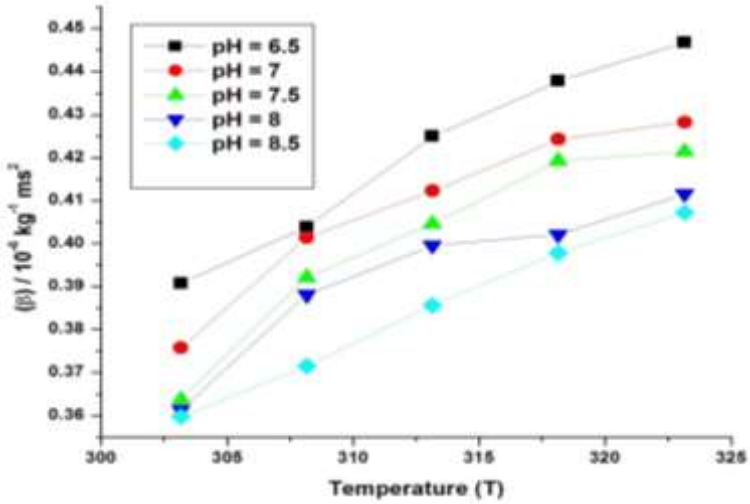

Figure 5: Variation of Adiabatic compressibility (β) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

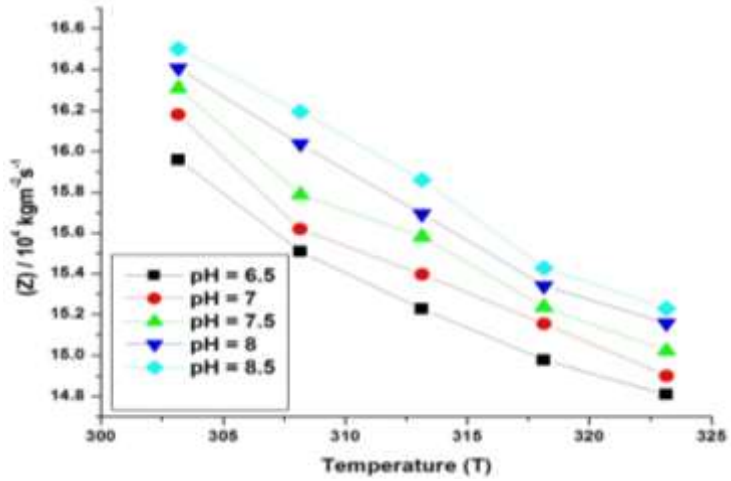

Figure 6: Variation of Specific acoustic impedance (z) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

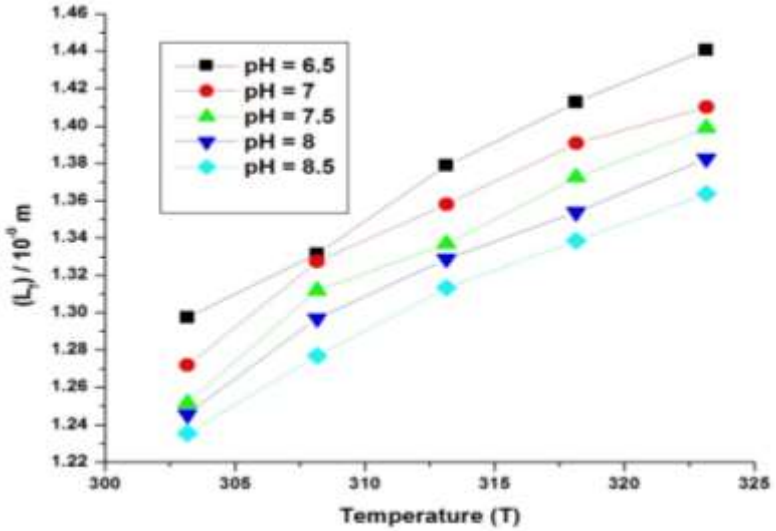

Figure 7: Variation of Intermolecular free length (L_f) for Paracetamol + Water at pH from 6.5 to 8.5 and at temperatures 303.15 to 323.15K at concentration 0.1 M

Table 2: Adiabatic compressibility (β), specific acoustic impedance (z) and intermolecular free length (L_f) for Paracetamol + Water system at pH from 6.5to 8.5 and at temperatures 303.15 to 323.15K

Concentration (M) = 0.1 M				
pH	**Temp. (K)**	**(β) / 10^{-6} kg^{-1} ms^2**	**(Z) / 10^4 $kgm^{-2}s^{-1}$**	**(L_f) / 10^{-9} m**
6.5	**303.15**	**0.3908**	**15.9594**	**1.2973**
	308.15	**0.4039**	**15.5097**	**1.3315**
	313.15	**0.4250**	**15.2275**	**1.3789**
	318.15	**0.4378**	**14.9770**	**1.4127**
	323.15	**0.4468**	**14.8093**	**1.4406**
7	**303.15**	**0.3757**	**16.1802**	**1.2718**
	308.15	**0.4014**	**15.6182**	**1.3273**
	313.15	**0.4123**	**15.3972**	**1.3581**
	318.15	**0.4243**	**15.1534**	**1.3908**
	323.15	**0.4283**	**14.9014**	**1.4103**
7.5	**303.15**	**0.3638**	**16.3101**	**1.2516**
	308.15	**0.3921**	**15.7882**	**1.3119**
	313.15	**0.4046**	**15.5817**	**1.3369**
	318.15	**0.4193**	**15.2368**	**1.3725**
	323.15	**0.4214**	**15.0215**	**1.3990**
8	**303.15**	**0.3614**	**16.4062**	**1.2456**
	308.15	**0.3881**	**16.0377**	**1.2969**
	313.15	**0.3996**	**15.6937**	**1.3288**
	318.15	**0.4021**	**15.3415**	**1.3539**
	323.15	**0.4116**	**15.1575**	**1.3827**
8.5	**303.15**	**0.3598**	**16.5015**	**1.2355**
	308.15	**0.3715**	**16.1961**	**1.2769**

	313.15	**0.3856**	**15.8611**	**1.3133**
	318.15	**0.3979**	**15.4288**	**1.3386**
	323.15	**0.4072**	**15.2296**	**1.3636**

IV. CONCLUSION

Ultrasonic investigation of molecular interaction in water soluble paracetamol has been carried out at a wide range of temperature and pH. The experimentally obtained parameters such as ultrasonic velocity, density, viscosity, refractive index and other acoustical parameters gives valuable information regarding molecular interaction present in solution. From experimental parameters it is conclude that there is molecular association takes place in the solution. Acoustic parameter shows that there is more force of interaction between solute and solvent by forming hydrogen bonding. This happened because there is more significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the solution .This may also specifies that increase in number of free ions showing the occurrence of ionic association due to stronger ion-ion interaction.

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