International Journal of Researches In Biosciences, Agriculture & Technology | Feb. 2015 Special Issue-1 | ISSN No. (Online) 2347-517X

Molecular Interaction of Aqueous Solution of Paracetamol at 2MHz and at Different Temperatures

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Abstract:

Ultrasonic velocity measurement plays an important role to study the interaction in the liquid and solutions. The measurement of ultrasonic velocity in liquid mixture gives valuable information about their physico-chemical properties and nature of molecular interaction in them. Paracetamol is an antipyretic drug which is used to reduce body temperature. Density and speed of sound of paracetamol drug was measured as a function of concentrations, temperatures. Adiabatic compressibility is used for detecting hydrogen bond formation in solutions. The Ultrasonic velocity, density and viscosity are measured experimentally. To study the nature and strength of molecular interaction in the aqueous solution of paracetamol, we have calculated the other related acoustical parameter such as adiabatic compressibility, internal pressure and Gibb's energy.

Key words: acoustic, adiabatic compressibility,ultrasonic, internal pressure

Introduction:

The study of propagation of ultrasonic waves in liquid systems and solids is powerful tool for examining certain physical properties of the materials. It is particularly well adapted to examining changes in such physical properties at the macro level. Many researchers have shown the important and fundamental role of the molecular details of the solvent species to determine the specific interactions[1-5] . Ultrasonic propagation parameters results with valuable information regarding the behaviour of binary liquid systems because of intramolecular and intermolecular association, dipolar interactions, complex formation and related structural changes affect the compressibility of the system which inturn produces corresponding variations in the ultrasonic velocity [6-7] Speed of sound itself is highly sensitive to the structure and interactions present in the liquid mixtures as it is fundamentally related to the binding forces between the constituents of the medium [8]. For the qualitative estimation of the molecular interactions in solutions, the ultrasonic velocity approach was first studied by Lageman[9].

In pharmacology, a drug is a chemical substance used in the treatment, cure, prevention, or diagnosis of disease or used to otherwise enhance physical or mental well-being. Drugs may be prescribed for a limited duration, or on a regular basis for chronic disorders[10].The paracetamol is antipyretic drug which is used to reduce body temperature. In continuation of our earlier work [11-14], in the present investigation we tried to study molecular interaction of aqueous paracetamol solution by measuring ultrasonic velocity, density and viscosity at 2MHzfrequency, and different temperatures. From the data acoustic parameters such as adiabatic compressibility, intermolecular free length and internal pressure were calculated.

The data and the results obtained during this investigation may give detail information regarding molecular interactions existing in the solution.

Experimental:

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 and viscosity measurements, in which continuous stirring of water was carried out with the help of electric stirrer and temperature variation was maintained within ±0.01^{0}C multi frequency interferometer (Mittal Enterprises, Model F-83) with accuracy of ±0.03% and frequency 2 MHz, was used in the present work for measurement of ultrasonic velocities of solutions. Densities of solutions were measured using specific gravity bottle. These values were accurate up to ± 0.1 kg/m^3. All the weighing was made on CA-124 (CB/CA/CT series, Contech) digital electronic balance having an accuracy of ± 0.0001g. Viscosities of the solution were measured by Ostwald's viscometer.

Result and discussion:

From the observed values the adiabatic compressibility, intermolecular free length and relaxation time was calculated.

Adiabatic compressibility was calculated by using the equation

$$\beta = 1/v^2.d \quad \ldots\ldots (1)$$

Intermolecular free length (L_f) has been evaluated from adiabatic compressibility (β) by Jacobson's formula,

$$L_f = K.\sqrt{\beta_s} \quad \ldots\ldots (2)$$

Expression for the determination of internal pressure Πi is

$$\Pi i = b.R.T.(K.\eta/U)^{1/2}.(\rho^{2/3}/Meff^{7/6}) \quad \ldots\ldots\ldots (3)$$

Gibbs free energy is calculated from the relation

$$\Delta G = K.T.\ln (K.T.\tau / h) \quad \ldots\ldots\ldots (4)$$

The values of acoustic and thermodynamic parameters for aqueous solution of paracetamol are tabulated in table 1, 2.

Table1 shows variation of ultrasonic velocity with temperatures. Ultrasonic waves are high frequency mechanical waves. Their velocities in a medium depend inversely on density and the compressibility of the medium reported by Hykes etal[15]. With increase in temperature ultrasonic velocity is increases. Addition of solute is indicative of greater association of molecules due to effective solute-solvent interaction which results increase in ultrasonic velocity. The oxygen atom of carbonyl group of paracetamol may associate with hydrogen atom of water molecule forming the hydrogen bond and hence velocity increases.

Table2 shows variation of adiabatic compressibility with temperatures. Adiabatic compressibility decreases with increasing temperatures. It is due to the influence of the electrostatic field of the ions on the surrounding water molecules

and solution becomes harder to compress. As temperature increases system becomes less compressible[16]. The decrease in adiabatic compressibility brings the molecules to a closer packing due to formation of hydrogen bond which shows strong solute –solvent interaction.

Table 3 shows variation of free length with temperatures. The decrease in free length may also due to the interaction of carbonyl group of paracetamol and water molecules and gets associated in the structure by electrostriction thus decreasing the free space available. The free length decreases due to compression which indicates the tight packing of the molecules so the intermolecular cohesion is strong leading to strong molecular associations this suggests that specific strong intermolecular interaction between paracetamol and water molecules existing in the solution. Decreased value of free length indicates structure promoting behavior of solute molecule.

In explaining molecular interaction, internal pressure plays an important role as it represents the resultant of the forces of attraction and repulsion between the molecules. It is found that internal pressure is decreasing with increase in temperature represents that there is strong interaction between the solute and solvent molecules. It may be due formation of thin or loose solvation layer. As observed solvation layer formed around paracetamol is may be hard. This shows that binding forces between the solute and solvent in liquid solution are becoming stronger which shows that there exists a strong molecular interaction.Gibbs' free energy increases slowly with increase of temperature. This may be the formation of hydrogen bonding in the solution.

Table. 1- Acoustic and thermodynamic parameters for aqueous solution of paracetamol at 2MHz

Temperature (K)	Ultrasonic Velocity (m/s)	Density (kg/ m^3)	Viscosity$x10^{-3}$ (kg $m^{-1}sec^{-2}$)
303.15	1490.05	1020.52	0.8391
308.15	1526.68	1015.44	0.7224
313.15	1563.03	1010.28	0.6606

Table. 2- Acoustical parameters of Paracetamol at different temperatures and at 2MHz.

Temperature (K)	Adiabatic Compressibility$\beta x10^{-10}$	Intermolecular free length (L_f)	Internal Pressure (Πi) x 10^5	Gibb's Free Energy (ΔG)$x10^{-20}$
303.15	4.41	0.0131	272.044	-7.173
308.15	4.23	0.0129	248.520	-7.322
313.15	4.05	0.0128	234.090	-7.460

Conclusion:

Ultrasonic studies have been carried out in aqueous solution paracetamol at different temperature at 2MHz. It is concluded that strong interaction exist in the solution.

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