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Ultrasonic Investigation of Molecular Interaction in Paracetamol Solution at Different Concentrations

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ABSTRACT
Paracetamol is an antipyretic drug, when it is taken it reduces the body temperature. So it was thought better to study intermolecular interaction and thus behavior of paracetamol under varied conditions such as temperature, concentration etc. For this certain important physical parameters such as adiabatic compressibility, specific acoustic impedance, relative association, intermolecular free length, relaxation time, free volume, Rao's constant, Wada's constant etc. are evaluated using ultrasonic velocity, density and viscosity of paracetamol solution at different concentrations and at 303K.

Key Words: Paracetamol, free volume, thermodynamic parameters, ultrasonic velocity.

INTRODUCTION

As gas is characterized by three variables such as temperature, pressure and volume liquid is characterized by parameters free volume, internal pressure and temperature. The associate nature of water with solute is learnt by its hydration Number [1]. While its structure making or breaking property is got from its free volume and internal pressure. To determine these parameters the ultrasonic velocity is a simple probe used by physicist along with basic quantities like density and viscosity [2].

The physico-chemical behavior and molecular interaction in pure liquid components and their mixtures is studied on the basis of acoustic and thermodynamic properties[3].The ultrasonic study is also useful to understand behavior of biomolecules [4]. Literature survey shows that ultrasonic study of liquid mixture is highly useful in understanding the nature of molecular interaction [5-7] and physicochemical behavior of liquid mixture[8-10].

In continuation of our work [11-12] in the present investigation the ultrasonic velocity, density and viscosity of 0.001 M, 0.01M and 0.1M paracetamol solution at temperature 303K is measured and acoustic and thermodynamic parameters have been calculated. From these parameters the effect of concentration on molecular interaction is interpreted.

EXPERIMENTAL SECTION

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 ± 0.01^0C Single crystal interferometer (Mittal Enterprises, Model F-81) 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 of 10 ml volume. These values were accurate up to ± 0.1 kg/m^3. All the weighing was made on Roy CCB-4 digital electronic balance having an accuracy of ± 0.001g. Viscosities of the solution were measured by Ostwald's viscometer.

RESULTS AND DISCUSSION

From the observed values the adiabatic compressibility, specific acoustic impedance, relative association, intermolecular free length, relaxation time, free volume, Rao's constant, Wada's constant were calculated.

Adiabatic compressibility was calculated by using the equation

$$\beta = 1/v^2.d \qquad \text{......(1)}$$

Where, v = velocity & d = density

Apparent molar compressibility (ϕK) can be calculated from the equation,

$$\phi K = [1000\,(\beta_s d_0 - \beta_0\, d_s) / m\, d_s\, d_0] + (\beta_s\, M/d_s) \qquad \text{......(2)}$$

Where, d_0 = density of pure solvent, d_s = density of solution, m = molality of solution M = molecular weight of solute, β_0 = adiabatic compressibility of pure solvent, and β_s = adiabatic compressibility of solution.

Specific acoustic impedance is determined from equations,

$$Z = v_s.d_s \qquad \text{......(3)}$$

Relative association is a function of ultrasonic velocity and is calculated by the equation,

$$R_A = \frac{d_s}{d_0}\left(\frac{v_0}{v_s}\right)^{1/3} \qquad \text{... ... (4)}$$

Where, v_0 and v_s are altrasonic velocities in solvent and solution respectively.

Intermolecular free length (L_f) is one of the important acoustic properties to study the intermolecular interactions. It has been evaluated from adiabatic compressibility (β) by Jacobson's formula,

$$L_f = K.\sqrt{\beta_s} \qquad \text{……(5)}$$

Relaxation time is calculated by following equation

$$\tau = 4/3\ \beta\eta \qquad \text{……(6)}$$

Free volume is calculated by following equation

$$V_f = \left(\frac{M_{eff}v}{K\eta}\right)^{3/2} \qquad \text{...... (7)}$$

Where, M_{eff} is effective molecular weight, K is a temperature independent constant which is equal to 4.28 x 10^9 for all liquids.

Rao's constant and Wada's constant is also a measure of interaction existing in the solution.

Rao's constant is calculated by using following equation.

$$R = [M_{eff}/d_s]v^{1/3} \qquad \text{……(8)}$$

Wada's constant is calculated by following equation.

$$W = [M_{eff}/d_s]\ ß^{-1/7} \qquad \text{……(9)}$$

The experimentally determine values are listed in table -1.

Increase in ultrasonic velocity with increase in concentration indicates that there is solute solvent interaction. Also increase in values of viscosity with increase in concentration confirmes that increase of cohesive forces because of strong interaction.

The adiabatic compressibility decreases with increase in concentration is shown in table- 2 indicates that there is strong solute solvent interaction. The solution is becoming more and more compressible. The similar behavior was observed by M. Aravinthaj etal[13] in study of acoustical and molecular interaction studies of amide with aliphatic amines in benzene at various temperatures.

Acoustic specific impedance increase with increase in concentration indicates that there is strong interaction between solute solvent.

Intermolecular free length decreases with increasing concentration shows that there is enhanced molecular association which is confirmed by values of viscosity which increases with concentration. Similar observation was made by P. S. Agrawal etal [14] in study of comparative study between acoustical nature and molecular interaction of copolymer and tetrapolymer.

Relative association is the measure of extent of association of the component in the mixture. The value of relative association decreases with increase in concentration indicating strong interionic interaction.

Table 1 :Ultrasonic Velocities, densities and viscosities of paracetamol Solution at 303K

Concentration of paracetamol (M)	Velocity (m/s)	Density (kg/ m^3)	Viscosityx10^{-3} (kg $m^{-1}sec^{-2}$)
0.001	1501.21	932.5	0.8279
0.01	1526.13	937.5	0.8495
0.1	1598.96	940.2	0.9122

Table 2: Acoustical parameter of paracetamol solution at 303K

Concentration of Paracetamol (M)	Adiabatic compressibility $\beta x10^{-10}$ (pa^{-1})	Specific acoustic impedance Zx 10^4 (kg $m^{-2}sec^{-1}$)	Inter molecular freelength L_f (A^0)	Relative association R_A	Acoustic relaxation time τ x 10^{-13}(sec)
0.001	4.7584	13.9987	0.1374	0.9837	5.2529
0.01	4.5797	14.3074	0.01350	0.9830	5.1876
0.1	4.1601	15.0334	0.01284	0.9122	5.0599

Table 3 : Thermodynamic parameters of paracetamol solution at 303K

Concentration of paracetamol (M)	Free volume V^f x 10^{-8} (m^3/mole)	Rao's constant R (m^3/mole)$(m/s)^{1/3}$	Wada's Constant W (m^3/mole)$(N/m^2)^{1/7}$
0.001	1.1953	2.213	4.144
0.01	1.2757	2.200	4.149
0.1	1.5491	2.268	4.245

Relaxation time decreases with increase in concentration. The relaxation time which is order of 10^{-12} sec is due to structural relaxation [15-16] process in such a case it is suggested that molecule get rearranged due to co-operative process[17] .

Free volume increases with increase in concentration, as shown in table-3, indicates that there is strong interaction between solute and solvent.

Rao's constant, also known as molar sound velocity, increases with increasing concentration shows that there is strong interaction between solute and solvent molecules.

Wada's constant also known as molar adiabatic compressibility may be considered for existing interaction. The values of Wada's constant increase with increasing concentration indicate that there must be tight packing of the medium and hence interaction is increasing. Thus there may be solute-solvent interaction occurring.

CONCLUSION

The acoustical and thermodynamic parameters calculated from measured properties suggest the strong molecular interaction in the solution. Ultrasonic investigations in aqueous solution of paracetamol at different concentrations give useful information in understanding interaction of solute with solvent.

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