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ULTRASONIC INVESTIGATION AS TOOL FOR STUDY OF MOLECULAR INTERACTION OF CEFTRIAXONE SODIUM AT DIFFERENT TEMPERATURES

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ABSTRACT

Acoustic is an active and important field of study that makes effective contribution to many areas of human endeavour. It relates to medicine, industry, music, art, architecture and life sciences. The thermodynamic and acoustical study with deals the nature of interactions between molecules in liquids and solutions. The study of propagation of ultrasonic waves in liquid system established as a simple and significant tool in determining the nature of interactions between molecules in liquids solution. In recent years ultrasonic measurements are found to be unique and nondestructive methods of determining the microstructures. Ultrasonic velocity, density and viscosity measurement have been carried out for 0.1 molar aqueous solution of ceftiaxone sodium at different temperatures and frequency 2 MHz. From this data various acoustical parameters are calculated which are used to predict molecular interaction present in the aqueous solution of ceftriaxone sodium.

Key words: Ultrasonic, Acoustic, Ceftriaxone sodium, Thermodynamic.

INTRODUCTION

The field of ultrasonic fairly vast and apart from day to day applications it is widely used in Medical Ultrasonic next to x-ray, non-destructive testing, acoustics in buildings, technological innovations in the field of ultrasonic continue to be translated into every day practice. Medical ultrasonic is now in period of rapid growth and is on verge of making a significant on clinical medicine. Ceftriaxone sodium is antibiotic used in pharmaceutical. Ultrasonic technique is used to study the nature of molecular interaction in liquids and liquid mixtures[1-2]. In continuation of our work[3-6] in the present investigation the ultrasonic velocity, density and viscosity of ceftriaxone sodium is measured and from these acoustical parameters such as adiabatic compressibility, acoustic impedance, intermolecular free length, relative association, relaxation time, free volume, Rao's constant and Wada's constant are determined.

EXPERIMENTAL

Antibiotic drug ceftriaxone sodium obtained from Prosperity 6 Pharmaceutics limited was used. Double distilled water was used for making solutions. Densities were measured with the help of density

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bottle. Weighing was done on Roy CCB-4 Balance, (± 0.001 g). A special thermostatic water bath arrangement was made for density, viscosity and ultrasonic velocity measurements in which there is continuous stirring of water with the help of electric stirrer and temperature variation was maintained within ± 0.1°C. All the ultrasonic velocities were measured by single crystal interferometer (Mittal Enterprises, Model F-81) with accuracy of ± 0.03% and frequency 2 MHz. The densities, viscosities and ultrasonic velocities of solvent water and 0.1 molar solution of ceftriaxone sodium were measured at 303.15, 308.15 and 313.15 K.

RESULTS AND DISCUSSION

In the present investigation, measurements of densities, viscosities and ultrasonic velocities of solvent water and an antibiotic cefotaxime sodium solution have been made and given in Table 1.

The adiabatic compressibility (β) is evaluated by using equation,

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

Specific acoustic impedance is determined from the measurement of ultrasonic velocity and density by formula,

$$Z = v_s . d_s \quad \ldots(2)$$

The solute-solvent interactions may be interpreted in terms of acoustic impedance.

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

$$RA = \frac{d_s}{d_0}\left(\frac{v_0}{v_2}\right)^{\frac{1}{3}} \quad \ldots(3)$$

Where, v_0 and v_s are ultrasonic velocities in solvent and solution.

Intermolecular free length (L_f) is one of the important acoustic properties to study the intermolecular interactions between the surfaces of molecules, on the other hand has a clear physical significance so it is used in defining free length.

Intermolecular free length has been evaluated from adiabatic compressibility (β) by Jacobson's[8] formula,

$$L_f = K\sqrt{\beta_s} \quad \ldots(4)$$

Where, K is the temperature dependent constant known as Jacobson's constant and is independent of the nature of liquid. (at 303.15 K, K = 631)

Relative Viscosity of Solution is calculated by equation,

$$\eta_2 = \eta_1.t_2.ds/t_1.d_0 \quad \ldots(5)$$

Where, η_2 = viscosity of experimental liquid, η_1 = viscosity of water, t_1 = time flow of water, t_2 = time flow of experimental liquid, d_0 = density of water and ds = density of experimental liquid.

Relaxation time is evaluated by equation,

$$\square = 4/3\beta.\eta \quad \ldots(6)$$

Where, β=adiabatic compressibility η = viscosity of experimental liquid

Free volume is calculated by following equation,

$V_f = [M_{eff}v/K \square]^{3/2}$ …(7)

Where, M_{eff} is effective molecular weight, K is a temperature independent constant which is equal to 4.28×10^9 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 equation,

$R = [M_{eff}/d_s]v^{1/3}$ …(8)

Wada's constant is calculated by equation,

$W = [M_{eff}/d_s]\ ß^{-1/7}$ …(9)

The experimentally determine values are listed in Table 1.

From this data molecular interaction in aqueous solution of ceftriaxone sodium will be predicted.

Table 1: Ultrasonic velocity, density and viscosity of aqueous solution of ceftriaxone sodium

Temperature (K)	Ultrasonic velocity(m/s)	Density(kg/m^3)	Viscosity*10^{-3} (N/m^2)
303.15K	1489.44	1054.37	0.9445
308.15K	1525.49	1044.61	0.9093
313.15 K	1598.64	1038.52	0.8508

Calculated adiabatic compressibility, acoustic impedance, relative association, intermolecular free length, relaxation time, free volume, rao's constant and wada's constant for aqueous solution of cefotaxime sodium at different temperatures are given in Table 2.

Table 2: Acoustic parameters of aqueous solution of ceftriaxone sodium at different temperature

Temperature (K)	β x 10^{-10} (pa^{-1})	Z x 10^4 (kg m^{-2}sec^{-1})	R_A	L_f (A^0)	τ x 10^{-10} (s)
303.15K	4.27	15.70	1.0696	0.01296	5.38
308.15K	4.11	15.93	1.0513	0.01271	4.99
313.15 K	3.77	16.60	1.0317	0.01217	4.27

Table 3: Thermodynamic parameters of aqueous solution ceftriaxone sodium at different temperatures

Temperature (K)	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)$^{1/7}$
303.15	1.61	0.2037	0.3889
308.15	1.74	0.2073	0.3947
313.15	1.84	0.2119	0.4020

From the table 1, it can be seen that the experimentally calculated values of density and viscosity of aqueous solution of ceftriaxone sodium decreases where as ultrasonic velocity increases with increases in temperature. The decrease values of density and viscosity with increase in temperature shows decrease in intermolecular forces due to increasing the thermal energy of the system. The increasing value of ultrasonic velocity with temperature shows strong attraction between the solute and solvent molecules.

From the Table 2 and 3, it reveals that the computed values of adiabatic compressibility, relative association and intermolecular free length decreases with increase in temperature shows that strong molecular interaction in aqueous solution of ceftrioxone sodium at higher temperature. At high temperature the acoustic impedance is increased which further support the possibility of molecular interaction between the solute and solvent molecules. The increase in the free volume shows that the strength of interaction increases gradually with the increase in temperature. It represent that there is strong interaction between the solute and solvent molecules. The increase in the values of rao's constant and Wada's constant with increase in temperature, which indicate the presence of strong molecular interaction.

Relaxation time decreases with increase in temperature. The relaxation time which is order of 10^{-12} sec is due to structural relaxation [7-8] process in such a case it is suggested that molecule get rearranged due to co-operative process.

The present investigation of aqueous solution of ceftriaxone sodium shows the agreement with the reported observations indicate solute-solvent interaction with intermolecular hydrogen bond between water molecule and ceftriaxone sodium molecule.

CONCLUSION

The computed acoustical parameters and their values point to the presence of strong molecular interaction in aqueous solution of ceftriaxone sodium. Hence it is concluded the molecular interaction in aqueous solution of ceftriaxone sodium is the of intermolecular hydrogen bonding in solution, which are responsible to drug absorption and transmission.

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