Experiments
Учебен експеримент в природните науки

ROLE OF ULTRASONIC WAVES TO STUDY MOLECULAR INTERACTIONS IN AQUEOUS SOLUTION OF DICLOFENAC SODIUM

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Abstract. Ultrasonic is a powerful nondestructive technique having wide range of applications in the field of material science. When ultrasonic wave passes through the medium these waves can actively interact with medium and activate the different processes in the medium. Structural changes occurring in the medium are explained in the form of velocity of propagation and amplitude of absorption. These two parameters are used as a function of temperature, pressure and frequency to evaluate several thermo acoustic parameters which gives detailed information about the molecular interaction. Ultrasonic velocity, density and viscosity measurements of Dichlofenac sodium in aqueous media have been made at different concentrations, temperatures and at different frequencies such as 2MHz, 4MHz and 6MHz. The data obtained during the investigation may give information regarding drug absorption, transmission and effect of the drug.

Keywords: ultrasonic wave, molecular interaction

Introduction

Ultrasonic is a powerful non-destructive technique. Ultrasonic study is very much useful for understanding the physicochemical properties of the liquids and various types of interactions in the solutions (Mirkar et al., 2011; Shinde et al., 2011; Shakya et al., 2011; Bhandakar et al., 2011; Punita & Uvarani, 2012). Ultrasonic wave propagation affects the physical properties of the medium and hence gives useful information about the molecular interactions in the liquid and liquid mixtures (Thiruwaran & Rajeswari, 2011). Knowledge of use of drug involving physiological and biochemical effects and their mechanism of action on macromolecules, sub cellular and organ system level can be studied in pharmokinetics (Rowland & Tozer, 1995; Gibaldi, 1991; Syal et al., 2005).

In continuation of our earlier work[1,2] (Aswale et al., 2007), in the present investigation we tried to study molecular interaction of aqueous Dichlofenac sodium solution by measuring ultrasonic velocity, density and viscosity at different frequencies, different

concentrations and different temperatures. From the data acoustic parameters such as adiabatic compressibility, intermolecular free length and relaxation time were calculated. The effect of frequency on the drug is interpreted.

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 $\pm 0.01^0$C. Multi frequency interferometer (Mittal Enterprises, Model F-83) with accuracy of ±0.03% was used in the present work for measurement of ultrasonic velocities of solutions at 2MHz, 4MHz and 6MHz. Densities of solutions were measured using specific gravity bottle with accuracy up to ± 0.1 kg/m^3. All the weighing was made on Roy CCB-4 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 formula

$$\beta = v^{-2}d$$

The intermolecular free length, L_f, was evaluated from the adiabatic compressibility,β, by using of Jacobson's formula

$$L_f = K\beta^{1/2}$$

And the relaxation time τ was calculated through

$$\tau = 4/3\beta\eta$$

At different frequencies, concentrations and temperatures the values of ultrasonic velocities, densities and viscosities are tabulated in Tables 1-3.

With increasing concentration and temperature ultrasonic velocity increases suggesting that solute solvent interaction is more. At 2MHz ultrasonic velocity increases at 303K for 0.01M while at 4MHzand 6MHz for 0.01m concentration the ultrasonic velocity decreases and at 313K at 4MHz ultrasonic velocity increases. Ultrasonic velocity increases linearly at 2MHz and 4MHZ at 313k but at 6MHz it shows non linearity. Increase in velocity shows that solute occupies the interstitial space of water and break the original state of water due to self-association. At 6MHz velocity decreases

Table 1. Acoustic parameters of aqueous solution of Dichlofenac sodium at 2MHz

Temperature (K)	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg/m^3)	Viscosity $\eta x10^{-3}$ (NSm^{-2})	Adiabatic compressibility $\beta x10^{-10}$	Intermolecular free length L_f (A^0)	Relaxation time $\tau x10^{-10}$
303.15	0.001	1524.48	1009.61	0.8215	4.26	0.0129	4.66
	0.01	1563.58	1020.58	0.8567	4.00	0.0125	4.57
	0.1	1601.30	1038.83	0.9642	3.75	0.0121	4.82
308	0.001	1492.57	1003.31	0.7378	4.48	0.0132	4.4
	0.01	1526.77	1014.72	0.7706	4.22	0.0129	4.34
	0.1	1564.25	1036.96	0.7957	3.94	0.0121	4.18
313	0.001	1454.82	1001.28	0.6783	4.72	0.0136	4.27
	0.01	1488.29	1008.85	0.6994	4.47	0.0132	4.17
	0.1	1526.12	1030.52	0.7550	4.16	0.0129	4.19

Table 2. Acoustic parameters of aqueous solution of Dichlofenac sodium at 4MHz

Temperature (K)	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg/m^3)	Viscosity $\eta x10^{-3}$ (NSm^{-2})	Adiabatic compressibility $\beta x10^{-10}$	Intermolecular free length L_f (A^0)	Relaxation time $\tau x10^{-10}$
303.15	0.001	1669.52	1009.61	0.8215	3.35	0.0118	3.89
	0.01	1593.80	1020.58	0.8567	3.85	0.0123	4.40
	0.1	1675.18	1038.83	0.9642	3.43	0.0116	4.41
308	0.001	1601.42	1003.31	0.7378	3.89	0.01236	3.82
	0.01	1598.74	1014.72	0.7706	3.855	0.0124	3.96
	0.1	1673.37	1036.96	0.7957	3.44	0.0117	3.65
313	0.001	1600.17	1001.28	0.6783	3.9	0.0123	3.52
	0.01	1670.85	1008.85	0.6994	3.55	0.0119	3.31
	0.1	1671.05	1030.52	0.7550	3.47	0.0118	3.50

with increasing concentration up to 0.01M means hydrogen bonding decreases while at 0.1M concentration velocity increases. Ultrasonic velocity decreases with increasing concentration and temperature suggest that available thermal energy used for breaking of bonds between the molecules. Thermal energy weakens the molecular forces which tend to decrease ultrasonic velocity. At high frequency ultrasonic velocity is highest for 0.001M solution at303K may be attributed to the cohesion brought about by ionic hydration in the solution. With increasing concentration viscosity increases as the solution become more viscous. As temperature increases the kinetic energy of the molecules and ions present in the solution increases and hence viscosity decreases.

Table 3. Acoustic parameters of aqueous solution of Dichlofenac sodium at 6MHz

Temperature (K)	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg/m^3)	Viscosity $\eta x10^{-3}$ (NSm^{-2})	Adiabatic compressibility $\beta x10^{-10}$	Intermolecular free length L_f (A^0)	Relaxation time $\tau x10^{-10}$
303.15	0.001	2298.32	1009.61	0.8215	1.87	0.0085	2.05
	0.01	2074.14	1020.58	0.8567	2.27	0.0094	2.60
	0.1	2181.2	1038.83	0.9642	2.02	0.0089	2.60
308	0.001	2295.33	1003.31	0.7378	1.89	0.00862	1.86
	0.01	2068.8	1014.72	0.7706	2.30	0.00958	2.30
	0.1	2182.49	1036.96	0.7957	2.02	0.0089	2.15
313	0.001	2290.08	1001.28	0.6783	1.9	0.00865	1.72
	0.01	2066.84	1008.85	0.6994	2.32	0.00968	2.16
	0.1	2179.7	1030.52	0.7550	2.04	0.0090	2.06

Adiabatic compressibility decreases with increasing concentration and temperature at 2 MHz, 4MHz and 6MHz which is shown in Fig. 1. The decreases in β values at these frequencies and increasing concentration shows that hydrogen bonding is strong between solute and solvent, there may be aggregation of solvent molecules around the solute molecules. The Dichlofenac sodium molecules are surrounded by layer of water molecules and firmly bound which increases internal pressure and hence decreases the adiabatic compressibility. At high concentration electrostatic forces causes the water structure to break and the solute surrounded water molecules are closely packed and hence compressibility decreases at high concentration.

Fig. 2 shows that the intermolecular free length decreases with increasing concentration and increases with increasing temperature at 2 MHz, 4MHz and at 6MHz. The low value of free length at 0.001M solution at 6MHz shows high value of ultrasonic velocity suggest that high dipole- dipole interaction which makes the system less compressible. The decrease value of compressibility brings the molecule to a closer packing resulting into a decrease of intermolecular free length. Free length decrease shows structure promoting behavior of solute.

Fig.3 shows that relaxation time is found to be decrease with increase in temperature and frequency and shows non linearity with increasing concentration. The non-linearity in relaxation time is due to change in concentration and temperature. The relaxation time decreases with increase in frequency indicates that bulk of cluster of solute around solvent decreases which shows strong interaction between solute and solvent molecules. The high value of relaxation time at 2MHz compared to 4MHz and 6MHZ suggest that there may be structural relaxation contribution at 2MHz. At 6MHz relaxation time has low value shows strong solute–solvent interaction.

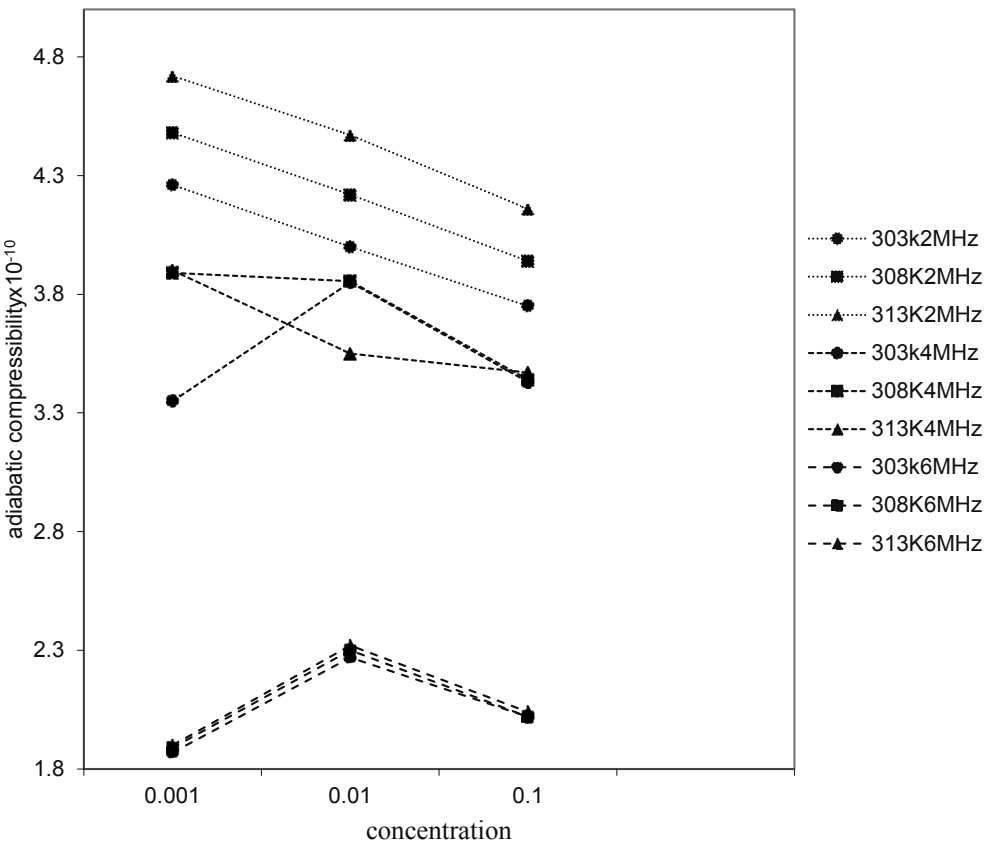

Fig 1. Adiabatic compressibility at different concentrations, temperatures and at different frequencies

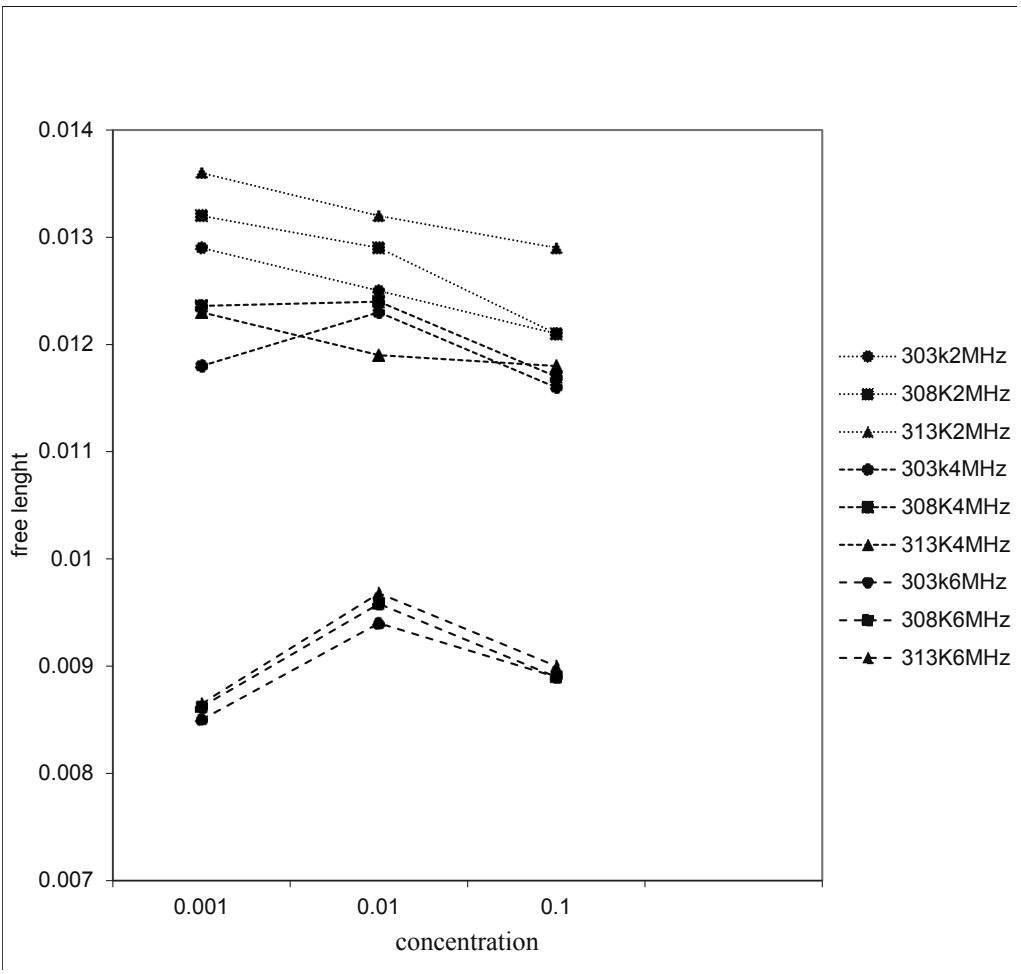

Fig 2. Free length at different concentrations, temperatures and at different frequencies

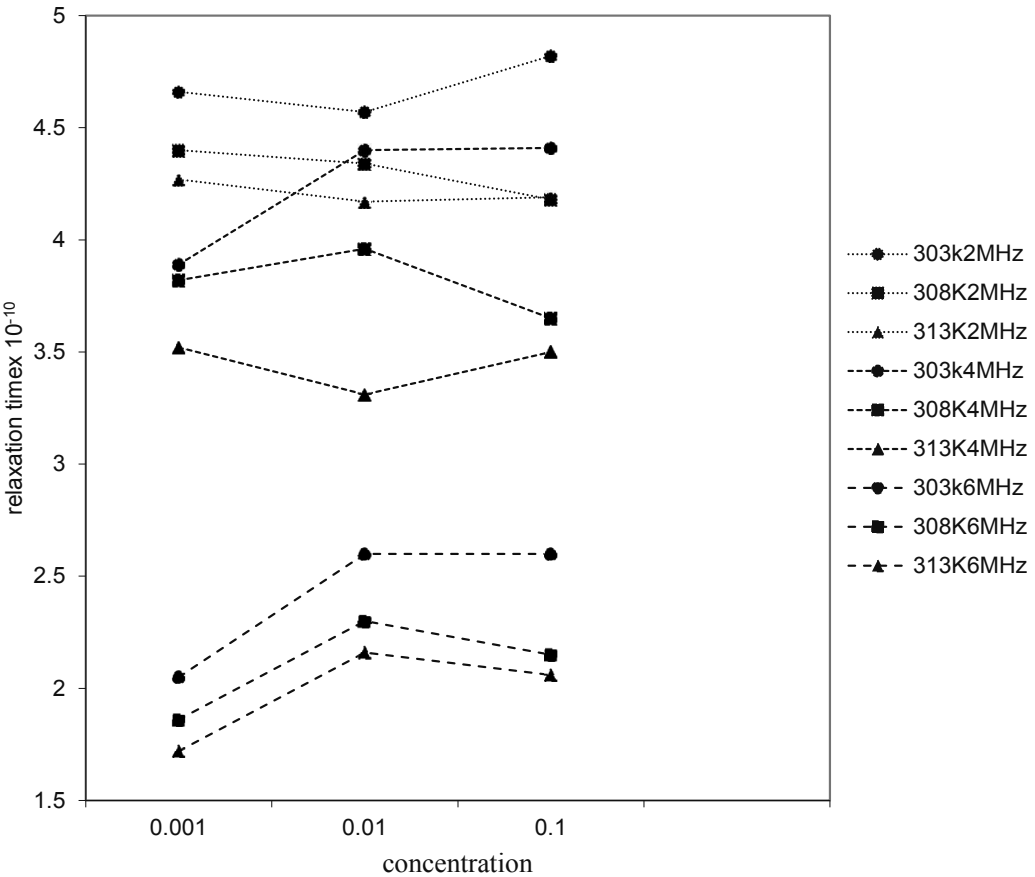

Fig 3. Relaxation time at different concentrations, temperatures and at different frequencies

NOTES

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