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Ultrasonic Velocity and Free Length of Aqueous Solution of Aspirin

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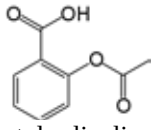
Abstract: ***Density and speed of sound of aspirin drug was measured as a function of concentrations, temperatures and frequencies. Many researchers suggested that adiabatic compressibility also used for detecting hydrogen bond formation in solutions. The Ultrasonic velocity and density are measured experimentally. In order to get more information on the nature and strength of molecular interaction, we have calculated the other related acoustical parameter such as adiabatic compressibility, specific acoustic impedance intermolecular free length, etc.***

Keywords: Ultrasonic frequencies, adiabatic compressibility, ultrasonic velocity, free length

1. Introduction

The values of densities, viscosities and ultrasonic velocities of liquids and liquid mixtures are essential to understand interaction between molecules. Ultrasonic study plays an important role to analyze physico-chemical behavior of molecular interaction[1-4]. To study the nature of the liquid state, it is very important to investigate the propagation of ultrasonic waves in pure liquids. The ultrasonic studies are extensively carried out to measure the thermodynamic properties and predict the molecular interaction of pure organic liquid. Moreover the ultrasonic velocity measurements have been successfully employed to detect and assess weak and strong molecular interactions present in binary and ternary mixtures. These parameters differ for various materials and also depend on the environmental conditions such as temperature[5-7].Utrasonic spectroscopy is concerned with the ultrasound attenuation and velocity across range frequencies. 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. When sound waves travel in different media change in the wavelength of sound speed takes place due to the elastic properties and induced particles vibrations. The density and sound speed measurement of certain dielectric liquids can be used to compute acoustical parameters like adiabatic compressibility, free length, acoustic impedance etc which gives information about the exact nature of molecular interactions among the components of solution.

Drug molecules in general are characterized by large hydrophobic groups, and are insoluble in water and therefore they are administered mostly in their salt form[8]. The solution behaviour therefore, depends upon the nature of solvent, functional groups, nature of drug and combination of different constituents forming the drug[8]. Taking the above view and in continuation of our earlier work[9-11] an attempt has been made to study the density and ultrasonic velocity measurements of analgesic drug in aqueous system in order to investigate various kinds of interactions that present in the solution. The structure of aspirin is as follows



. Acetyl salicylic acid

2. 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% and frequency 2 MHz, 4MHz, 6MHz were 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.

3. 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

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

Specific impedance has been calculated by using the equation

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

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

$$L_f = K.\sqrt{\beta_S} \quad \ldots\ldots.. (3)$$

The values of acoustic and thermodynamic parameters for aqueous solution of paracetamol at different frequencies are tabulated in table 1, 2, 3.

Table 1: Thermodynamic parameters of Aspirin at 2 MHz

Temperature (K)	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg/m^3)	Adiabatic compressibility $\beta x 10^{-10}$	Specific acoustic impedance $Zx10^4$ ($Kgm^{-2}sec^{-1}$)	Intermolecular free length L_f (A^0)
303.15	0.001	1475.75	1020.74	4.498	15.0635	0.01329
	0.01	1529.17	1022.17	4.18	15.6307	0.01282
	0.1	1564.86	1024.98	3.984	16.0395	0.01251
308.15	0.001	1493.38	1019.73	4.397	15.2284	0.01324
	0.01	1530.66	1020.07	4.18	15.6138	0.01291
	0.1	1527.23	1022.67	4.192	15.6185	0.01293
313.15	0.001	1526.21	1017.02	3.923	15.5218	0.01306
	0.01	1563.78	1019.67	4.01	15.9454	0.01273
	0.1	1528.47	1021.87	4.18	15.6189	0.01301

Table 2: Thermodynamic parameters of Aspirin at 4MHz

Temperature (K)	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg/m^3)	Adiabatic compressibility $\beta x 10^{-10}$	Specific acoustic impedance $Zx10^4$ ($Kgm^{-2}sec^{-1}$)	Intermolecular free length L_f (A^0)
303.15	0.001	1669.58	1020.74	3.51	17.0420	0.0117
	0.01	1678.29	1022.17	3.47	17.1549	0.01186
	0.1	1673.00	1024.98	3.48	17.1479	0.01117
308.15	0.001	1679.29	1019.73	3.477	17.2138	0.0117
	0.01	1670.45	1020.07	3.51	17.0397	0.0118
	0.1	1676.98	1022.67	3.47	17.1490	0.0117
313.15	0.001	1677.38	1017.02	3.49	17.0592	0.0117
	0.01	1666.93	1019.67	3.53	16.9971	0.0118
	0.1	1673.92	1021.87	3.492	17.1052	0.0117

Table 3: Thermodynamic parameters of Aspirin at 6MHz

Temperature (K)	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg/m^3)	Adiabatic compressibility $\beta x 10^{-10}$	Specific acoustic impedance $Zx10^4$ ($Kgm^{-2}sec^{-1}$)	Intermolecular free length L_f (A^0)
303.15	0.001	1753.2	1020.74	3.18	17.8956	0.0111
	0.01	1749.31	1022.17	3.20	17.8809	0.01121
	0.1	1744.80	1024.98	3.24	17.8838	0.01122
308.15	0.001	1744.71	1019.73	3.22	17.7913	0.01133
	0.01	1742.22	1020.07	3.23	17.7718	0.01134
	0.1	1740.24	1022.67	3.22	17.7969	0.01134
313.15	0.001	1746.63	1017.02	3.223	17.7635	0.01141
	0.01	1740.82	1019.67	3.23	17.7506	0.0114
	0.1	1738.01	1021.87	3.239	17.7602	0.01144

With increasing frequency ultrasonic velocity increases, but with increasing concentration and temperature it shows non linearity. At 2MHz and at 303.15K ultrasonic velocity increases while at 4MHz for 0.1M it decreases and at 6MHz ultrasonic velocity decreases with increasing concentration and temperature. The increase in concentration weakens the molecular forces and hence change in velocity is observed. It is due to significant interaction between ions and solvent molecules suggesting structure promoting behavior of added solute. It also indicates that availability of free ions is less due to weak ion-ion interaction and hence velocity decreases at 6MHz. At 2MHz at 308.15K and 313.15K, velocity increases up to 0.01M and then decreases while at 4MHz velocity decreases up to 0.01M and then increases. Increase in ultrasonic velocity for 0.01M at 2MHz and for 0.1M at 4MHz at 308.15K, 313.15K shows structure breaking effect of solute which disrupt the water structure. This could be followed by structural reorganization leaving the molecules in fitting helical cavities[12]. This may cause an increase in closed packed structure which increases cohesion between water molecules, resulting solution less compressible and velocity increases. It indicates solute-solvent interaction existing in the solution.

Density increases with increasing concentration and decreases with rise in temperature. Increase in density with increase in concentration is due to shrinkage in the volume which in turn due to presence of solute molecules. In other words increase in density may be interpreted to the maker of solvent due to added solute[13]. It indicates solute-solvent interaction.

Fig.1 shows variation of adiabatic compressibility with concentration, temperature and frequency. Increase in frequency decreases adiabatic compressibility. At 2MHz, 303.15K β decreases while at 4MHz for 0.1M it slightly increases and at 6MHz it increases .At 308.15K and 313.15K for0.1M at2MHz β increases and at 4MHz, 6MHz

for 0.01M adiabatic compressibility increases and then decreases. Decrease in adiabatic compressibility at 2MHz at 303.15K shows strong interaction between solute and solvent molecules. At 4MHz, 6MHz at high temperature for 0.01M adiabatic compressibility increases. It may due to collection of solvent molecules around the solute ions indicating weak ion-solvent interaction. This suggests that there is significant solute-solvent interaction. The increase in adiabatic compressibility following a decrease in ultrasonic velocity shows weakening of intermolecular interaction[14]. For 0.1M solution there is larger probability of aspirin molecules forming hydrogen bond with water molecules. The intermolecular forces are strong which breaks the cluster of water by solute by solute molecules resulting in enhancing the closed packed structure of solvent and hence adiabatic compressibility decreases. It suggests the structure promoting of solvent while at 0.01m adiabatic compressibility increases shows structure breaking effect.

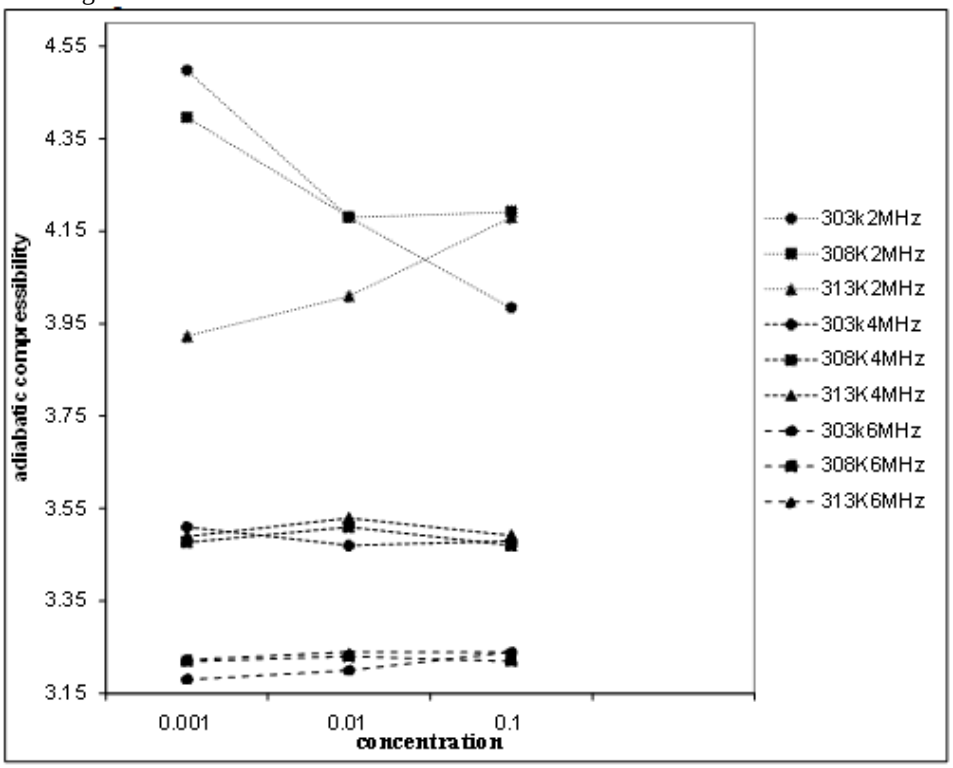


Figure 1: adiabatic compressibility at different concentration, temperature and frequencies.

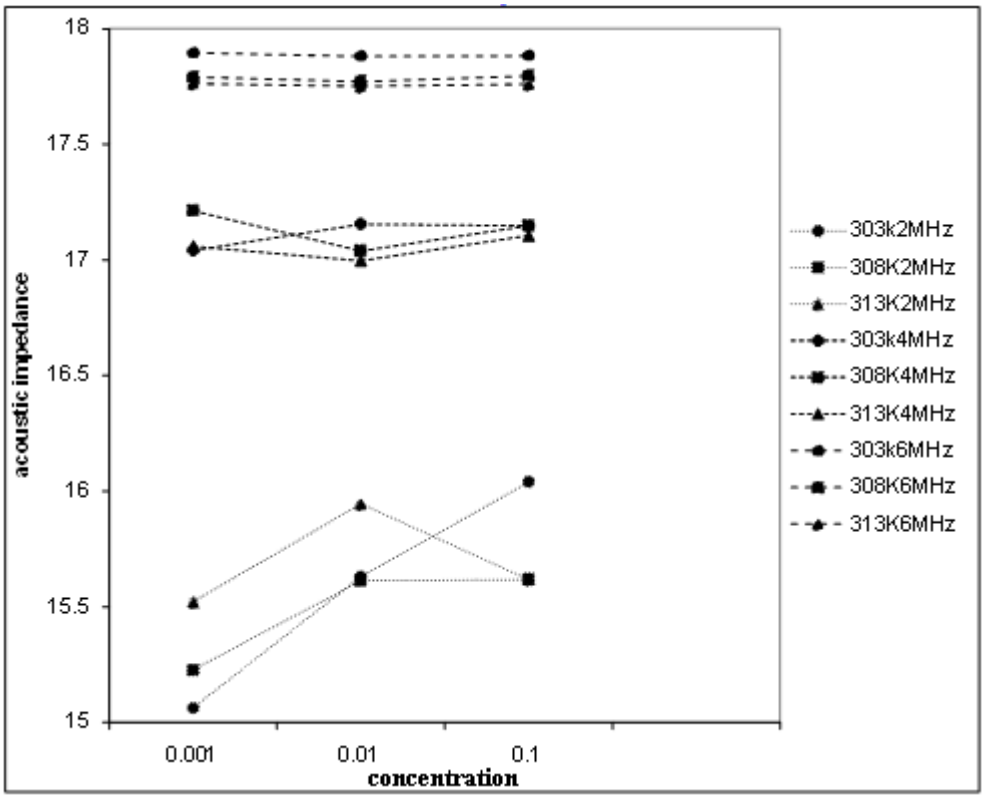


Figure 2: Acoustic impedance at different concentration, temperature and frequencies.

Fig.2 shows variation of acoustic impedance with concentration, temperature and frequency. Specific acoustic impedance increases with increasing concentration, temperature and frequency. Kinsler etal[15] have suggested that acoustical impedance is more significant parameter to describe the medium and intermolecular interactions than the ultrasound velocity and density individually. At 2MHz at all temperature Z increases while at 4MHz and 6MHz it varies non linearly. At high frequency and at high temperature Z decreases for 0.01M and then increases for 0.1M solution. Increase in Z may be due to closeness of solute particle and increasing existing in the solution.

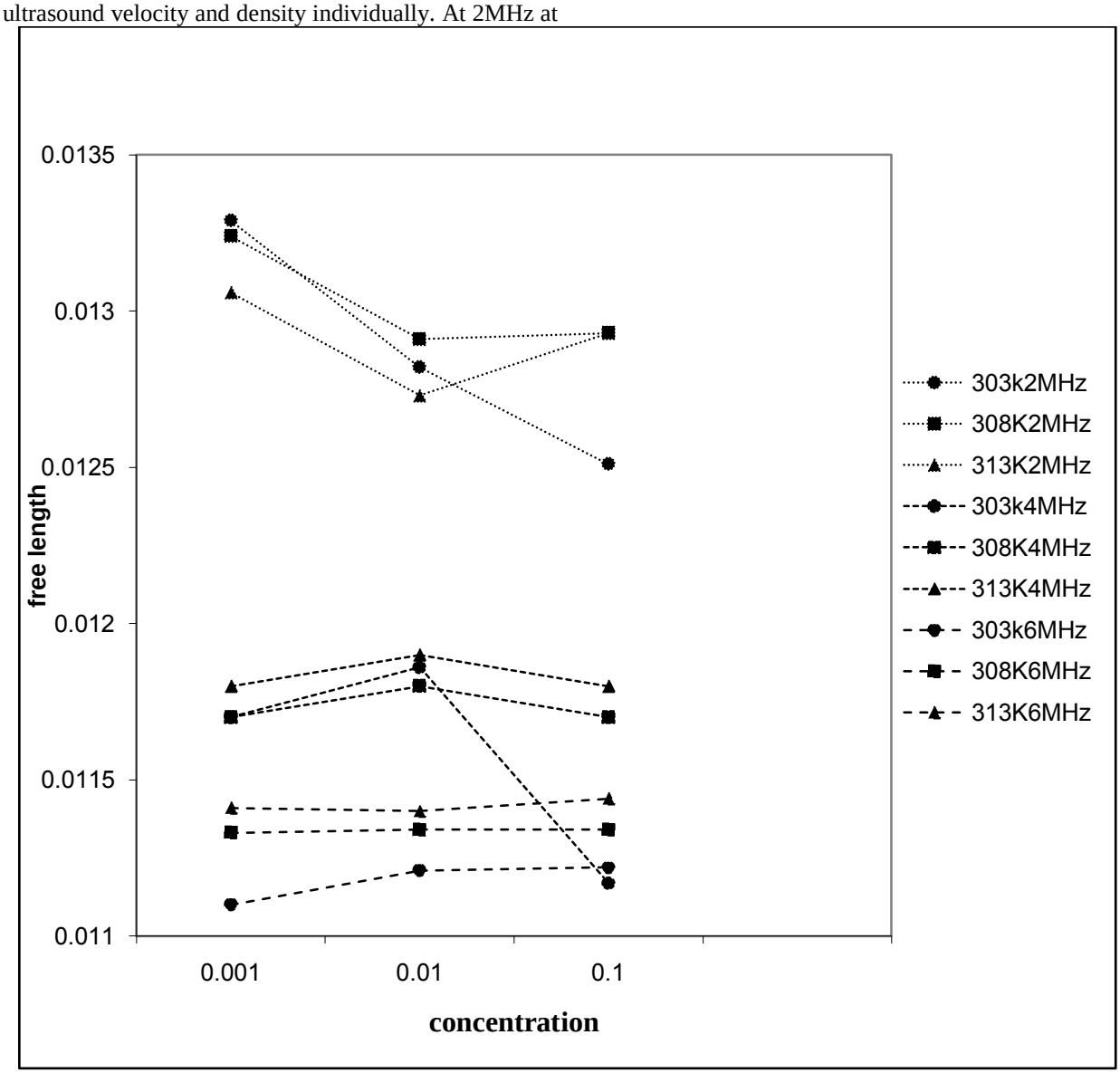


Figure 3: Free length at different concentration, temperature and frequencies.

Fig.3 shows variation of free length with concentration, temperature and frequency. The free length is found to be a predominant factor for determining the nature of ultrasonic velocity in liquid mixtures. Intermolecular free length is the mean distance between the surfaces of neighboring molecule. Free length decreases with increasing frequency. But a 4MHz, 6MHz it shows non linearity with increasing concentration and temperature. Decrease in L_f shows strong interaction between solute-solvent.

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