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Acoustic Study of Molecular Interactions in some Aqueous Antimicrobials at 298K

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Abstract: ***The behaviour of aqueous solutions of some antimicrobial at different molar concentrations is analyzed by studying the variation of ultrasonic velocity, adiabatic compressibility, free length and internal pressure. These measurements were carried out by using the ultrasonic pulse echo overlap (PEO) technique at a frequency of 5 MHz at temperature 298K. The values of these thermodynamic parameters show non-linear behaviour with increase in molar concentration of antimicrobials. This shows the presence of molecular interactions, complex formation, formation of hydrogen bonds, solute-solvent interactions in the antimicrobial solution.***

Keywords: Ultrasonic velocity, thermodynamic parameters, molecular interactions.

1. Introduction

The study of propagation of ultrasonic waves in liquid and liquid mixtures provide a wealth of information about the state of the liquid. The measurement of ultrasonic velocity in liquid mixtures is an important tool to study the physico-chemical properties of the liquid and also explains the nature of molecular interactions [1-3]. The present study is undertaken with a view to find the nature of solute-solvent interactions and to find out the influence of conformational features over ultrasonic velocity at temperature 298K.

2. Experimental Details

In the present study, three pure antimicrobials viz; Amoxicillin (trihyd.), Cephalexin, Ciprofloxacin (HCl) were procured from the different pharmaceutical companies. A solution of 0.01 molarity was prepared . The ultrasonic velocity was measured at 5MHz by using an automatic ultrasonic attenuation recorder (AUAR-102) and a frequency counter APLAB-1116. The density and viscosity of the solution were measured by hydrostatic sinker method and Ostwald's viscometer respectively. For the measurement of ultrasonic velocity, a specially designed and fabricated stainless steel cell was used. All the measurements were made at constant temperature range 25± 0.1^{O}C by circulating water from a thermostatically controlled water bath. (thermostate U-10).

3. Results and Discussion

The measured values of ultrasonic velocity, density, viscosity and other computed parameters namely adiabatic compressibility, free length and internal pressure of aqueous antimicrobials viz; Amoxycillin (trihyd.), Cephalexin, Ciprofloxacin (HCl) in the different concentration range are given in tables 1-3; and the results for all three antimicrobials have been represented in figures 1-3. It is found that in aqueous Amoxycillin solution the parameters ultrasonic velocity (u), adiabatic compressibility (β_a), internal pressure (P_i) and free length (L_f) show non-linear variations with increasing molar concentration. The ultrasonic velocity exhibits a peak at 0.0002M while internal pressure exhibits non-linear decrease with molar concentration (Fig. 1a & 2a) on the other hand there is a significant dip in ultrasonic velocity at 0.0006M (Fig. 1a) while adiabatic compressibility and free length show similar trends with a significant peak at the same concentration (Fig. 1a & 3a). In aqueous Cephalexin, adiabatic compressibility and free length show similar non-linear behaviour with increasing molar concentration exhibiting two dips at 0.0001M and 0.0008 M (Fig. 1b, 3b) while ultrasonic velocity exhibits two peaks at the same concentration (Fig. 1b). The variation of internal pressure exhibits a peak at 0.0001M and a slight dip at 0.0008M (Fig. 2b). In aqueous Ciprofloxacin, the variation of ultrasonic velocity exhibits a peak at 0.0001M and a dip at 0.0006M (Fig. 1c), while the variation in adiabatic compressibility and free length is slight similar with significant dip at 0.0001M then there is no significant change in their nature with increasing molar concentration (Fig. 1c & 3c). The internal pressure shows significant dip at 0.0001M and peak at 0.0002M (Fig. 2c), thereafter with the addition of drug there is a gradual increase in internal pressure.

The non-linear behaviour of acoustic and thermodynamic parameters can be used to deduce information about the liquid systems. The non-linearity confirms the presence of complex formation, solute-solvent interaction [4] and weak association due to hydration [5]. The non-linearity between ultrasonic velocity and the solute concentration may be attributed to the association due to the antimicrobial molecules and water molecules. The probability of hydroxyl groups of water molecules are large and this leads to the formation of hydrogen bonds and thereby increases cohesion resulting in a significant increase of ultrasonic velocity. The decrease in the value may be due to the weakening of intermolecular forces due to formation of strong bonds. The variation of adiabatic compressibility with solute concentration may be attributed to the structural changes taking place in the solvent water [6,7] and these changes are generally large due to the addition of solute, which optimizes the structural changes at the solute concentration

where peaks are observed. An increase in compressibility indicates less cohesive nature of the medium [8] while the decrease in compressibility at particular concentration indicates the enhancement of degree of association [9] due to the larger possibility of formation of hydrogen bonding in between drug molecules and water i.e. increase in cohesion.

In all the three systems the internal pressure is found to increase or decrease with molar concentration. The increase in internal pressure shows the orientation of the solvent molecules around the ions COO^- and NH_3^+ present in the solution and this may be due to the influence of electrostatic field of ions. This indicates the association tendency of the molecules while decreasing internal pressure at some concentration indicates the dissociating tendency of the molecules in binary solutions. The non-linear trends in free length indicate the presence of specific interactions between the component molecules [10].

Thus, the behaviour of ultrasonic velocity, adiabatic compressibility, internal pressure and free length provide an insight into the molecular interactions of antimicrobials and water molecules.

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Table 1: Acoustical parameters for aqueous Amoxycillin (trihyd.) at 298 K

C_m	ρ gm-cm^{-3}	u cm-sec^{-1}	η_s Cp	$ß_a$ x 10^{-11} cm^2/dyne	L_f x 10^{-11} cm	P_i x 10^8 dyne /cm^2
0.0000	0.9971	149608	0.893700	4.4809	4.1837	2.7138
0.0001	0.9969	149658	0.893250	4.4787	4.1827	2.7053
0.0002	0.9965	149698	0.892625	4.4779	4.1823	2.6963
0.0003	0.9974	149670	0.895625	4.4759	4.1814	2.6956
0.0004	0.9977	149639	0.897251	4.4762	4.1815	2.6920
0.0005	0.9973	149613	0.896825	4.4795	4.1831	2.6840
0.0006	0.9970	149590	0.896500	4.4821	4.1843	2.6763
0.0007	0.9973	149748	0.898250	4.4713	4.1792	2.6712
0.0008	0.9975	149785	0.900249	4.4684	4.1779	2.6673
0.0009	0.9976	149805	0.901751	4.4667	4.1771	2.6627
0.0010	0.9977	149820	0.902950	4.4655	4.1765	2.6577

Table 2: Acoustical parameters for aqueous Cephalexin at 298 K

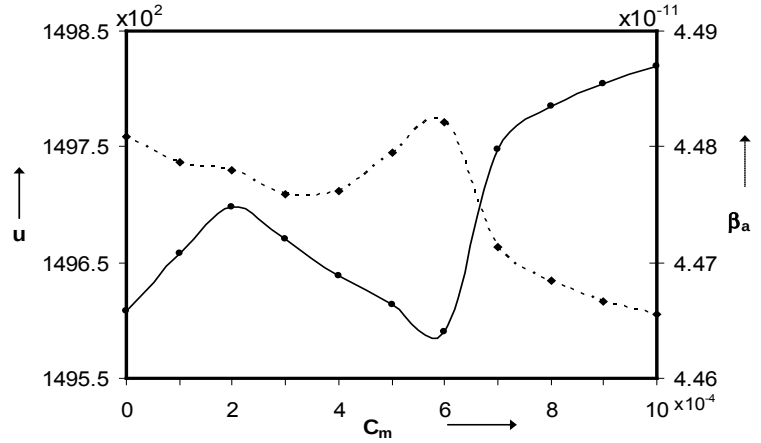
C_m	ρ gm-cm^{-3}	u cm-sec^{-1}	η_s Cp	$ß_a$ x 10^{-11} cm^2/dyne	L_f x 10^{-11} cm	P_i x 10^8 dyne /cm^2
0.0000	0.9971	149608	0.893700	4.4809	4.1837	2.7138
0.0001	0.9977	149780	0.902275	4.4679	4.1776	2.7202
0.0002	0.9978	149766	0.901750	4.4680	4.1777	2.7137
0.0003	0.9979	149736	0.901500	4.4694	4.1784	2.7077
0.0004	0.9979	149718	0.902110	4.4704	4.1788	2.7028
0.0005	0.9979	149823	0.903050	4.4640	4.1758	2.6973
0.0006	0.9981	149891	0.901875	4.4592	4.1736	2.6892
0.0007	0.9983	149926	0.900175	4.4564	4.1723	2.6806
0.0008	0.9984	149956	0.899000	4.4541	4.1712	2.6729
0.0009	0.9983	149910	0.902050	4.4574	4.1727	2.6717
0.0010	0.9982	149864	0.903675	4.4607	4.1743	2.6684

Table 3: Acoustical parameters for aqueous Ciprofloxacin (HCl) at 298 K

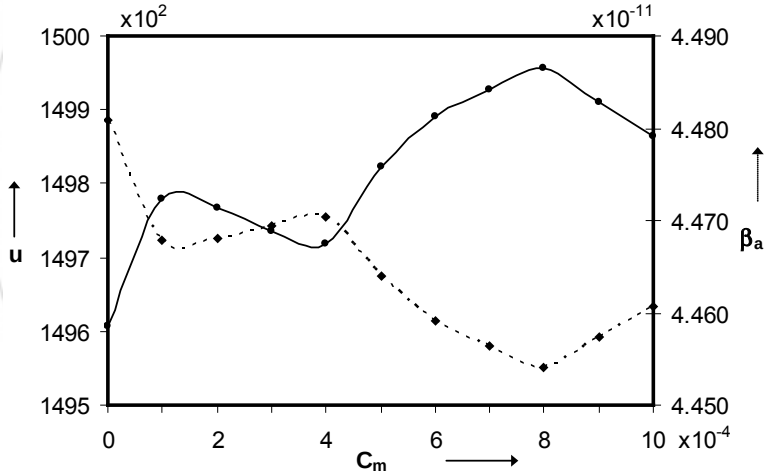
C_m	ρ gm-cm^{-3}	u cm-sec^{-1}	η_s Cp	$ß_a$ x 10^{-11} cm^2/dyne	L_f x 10^{-11} cm	P_i x 10^8 dyne /cm^2
0.0000	0.9971	149608	0.893700	4.4809	4.1837	2.7138
0.0001	0.9985	149851	0.880210	4.4600	4.1739	2.6872
0.0002	0.9979	149840	0.945620	4.4631	4.1754	2.7777
0.0003	0.9986	149810	0.930616	4.4622	4.1750	2.7505
0.0004	0.9988	149800	0.927420	4.4618	4.1748	2.7398
0.0005	0.9991	149772	0.927430	4.4616	4.1747	2.7343

0.0006	0.9995	149744	0.930112	4.4620	4.1749	2.7326
0.0007	0.9993	149775	0.955042	4.4607	4.1743	2.7620
0.0008	0.9992	149825	0.961992	4.4584	4.1732	2.7647
0.0009	0.9990	149840	0.966040	4.4584	4.1732	2.7636
0.0010	0.9988	149850	0.992060	4.4586	4.1733	2.7936

C_m = Antimicrobial concentration, **ρ**=Density of the solution**, u** = Ultrasonic velocity**,**
η_s = Shear viscosity, **ß$_a$** = Adiabatic compressibility, **L_f** = Free length and **P_i** = Internal pressure.



(a)



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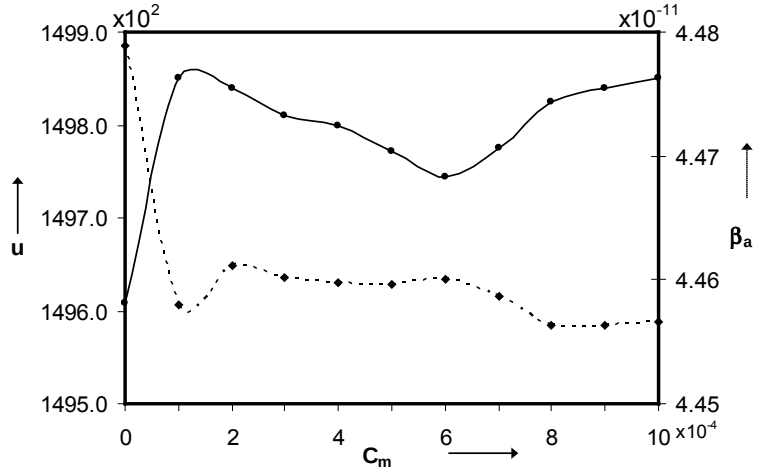
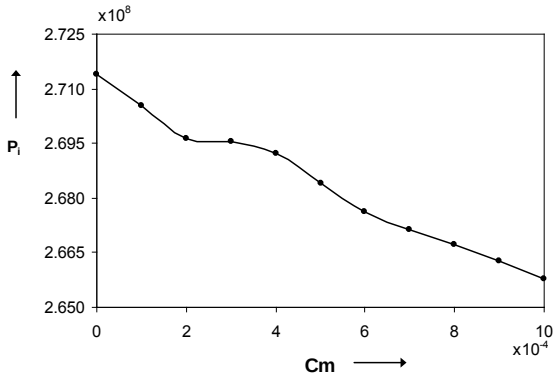
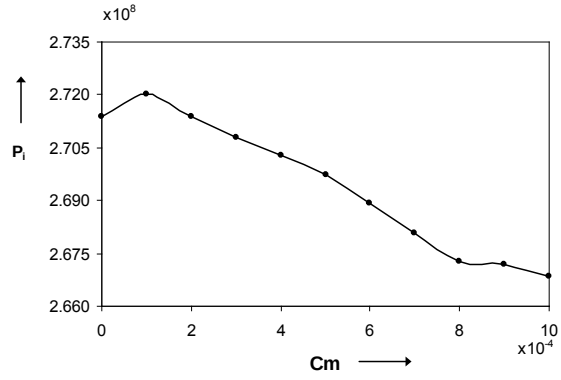


(c)

Figure 1: Variation of ultrasonic velocity (u) and Adiabatic compressibility (β_a) with molar concentration (C_m) in aqueous (a) Amoxycillin (trihyd.), (b) Cephalexin , (c) Ciprofloxacin (HCl).



(a)



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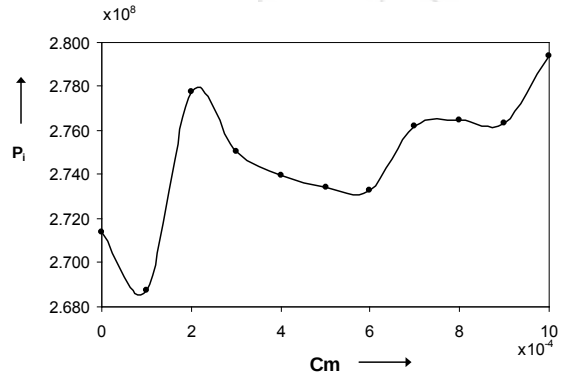
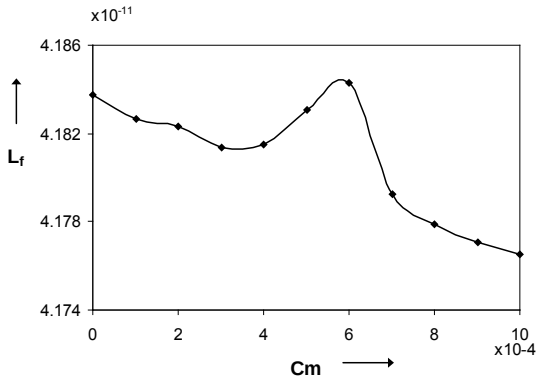
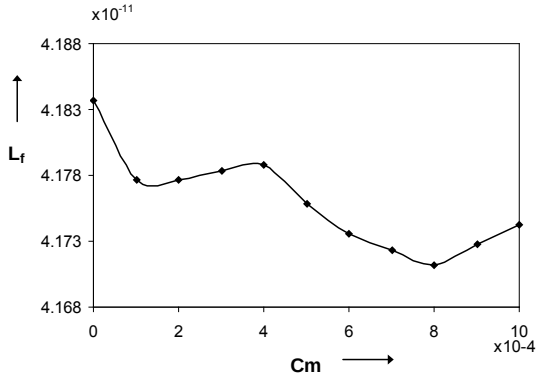


(c)

Fig. 2 : Variation of internal pressure (Pi) with molar concentration (C_m) in aqueous (a) Amoxycillin (trihyd.), (b) Cephalexin and (c) Ciprofloxacin (HCl).



(a)



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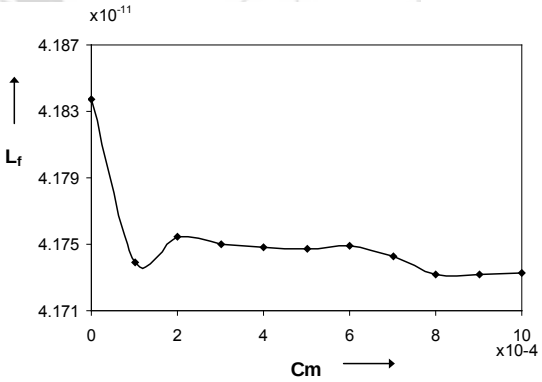

(c)

Fig. 3 : Variation of free length (Lf) with molar concentration (C_m) in aqueous (a) Amoxycillin (trihyd.), (b) Cephalexin and (c) Ciprofloxacin (HCl).