ULTRASONIC STUDIES OFMOLECULAR INTERACTIONS IN THE SOLUTION OF ANTIMALARIALDRUG AT 318K

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Abstract
Chloroquine phosphate is an antimalarial and amebicidal drug.In the present study ultrasonic velocity (U), density (ρ) and viscosity (η) have been measured at frequency 2 MHz in the binary mixtures.The measured value of ultrasonic velocity, density and viscosity have been used to estimate the acoustical parameters namely adiabatic compressibility (βa), relaxation time (τ), acoustic impedance (z), free length (Lf), free volume (Vf) and internal pressure (Pi),Wada's constant(W), Rao's constant (R) to investigate the nature and strength of molecular interaction in the binary mixture with water. The obtained results support the occurrence of complex formation, molecular association through intermolecular hydrogen bonding in the binary liquid mixtures.
Key Words:Ultrasonic velocity,chloroquine phosphate drug, molecular interaction

Introduction

Ultrasound refers to sound waves of such a high frequency that it cannot be heard. High resolution ultrasound imaging has been used for determination of melanoma invasion depth in vivo for preoperative staging purposes [1-2]. Now a days ultrasonic technology is employed in a wide range of applications in medicine, biology, industry, material science, agriculture, oceanography, sonochemistry research etc. due to its non-destructive nature[3-10]. These waves have also been used to extract and release intracellular enzymes such as invertase, to promote enzyme release, enhance productivity in biological processes [11] etc. In field of agriculture, ultrasound waves have been utilized extensively in chemical additives (fertilizers and plant protection preparations) for improving the production yield of food produced. In material chemistry, ultrasound waves have been useful in the preparation of biomaterials, protein microspheres, in the modification of polymers and polymer surfaces etc. [12-17]. Much work has been done in solutions of polymers [18-23] , amino acids [24-25] and other electrolytes [26-33] .The acoustic waves with frequencies of about 20 KHz and above are known as ultrasonic waves.The velocity of sound in air and liquid is 330m/s and 1200m/s respectively**.**The shortest ultrasonic waves therefore have wave length of the order of visible light.The measurement of ultrasound refers to sound waves of such a high frequency that it cannot be heard. The measurement of sound velocity is simple in ultrasonic wavesand therefore velocity measurement in small amount of samplecan be determined very accurately and easily.In the recent years,ultrasonic waves have acquired status of an important probe,for the study of structures and properties of matter.In the field of technology,the waves are being used for detectionof flaws,testing of material,mechanical cleaning of surface etc.In basic science they are used to provide information about the behavior of themicroscopic particles of matter.The observation and dispersion of ultrasonic wave provides information on the relaxation process and molecular interaction in the liquid.Such information is of very importance for the understanding of the liquid state.A large amount of work has been done on the absorption of ultrasonic waves in liquid.The study of ultrasonic waves in binary mixture of liquid shows the ultrasonic wave velocities and their derived excess parameters can be used to determined the relative strength of homo and hetero-moleculer interaction in it.The above mentioned application of ultrasonic waves in basic science and technology are primarily due to their dependence on molecular structures and types of constituents in the medium.The ultrasonic wave velocity in number of liquids thus differs according to its purity [34-38].

Materials and Methods

The ultrasonic velocity(U) have been measured on ultrasonic interferometer Mittal Model-F-05 with an accuracy of 0.1%.The viscosities (η) of binary mixtures were determined using Ostwald's viscometer by calibrating with double distilled water with an accuracy of ±0.001 Pa. Sec. The density (ρ) of these binary solution was measured accurately using 25 ml specific gravity bottle in an electronic balance precisely.Before measuring the velocity of particular sample, the interferometer was adjusted and its accuracy was determined.For this,water and Chloroquine phosphate binary mixture was taken in the measuring cell,for the purpose of calibration of instrument.The current in the micro-ammeter was adjusted to 40μA for maximum deflection and suitable adjustments were made for the minimum.Theultrasonic velocity was calculated .The frequency of ultrasonic wave is 1MHz.

1.Ultrasonic velocity (υ): The relation used to determine the ultrasonic velocity is given by

$\upsilon = f \times \lambda \ ms^{-1}$

Where, f - Frequency of ultrasonic waves, λ - Wave length

2. Adiabatic compressibility (κ): Adiabatic compressibility which is defined as,

$\kappa = (1/\upsilon^2 \rho) \ \ kg^{-1} ms^2$

Where, υ – Ultrasonic velocity, ρ – Density of the solution

3. Free volume (V_f): Free volume in terms of the ultrasonic velocity (υ) and the viscosity of the liquid (η) calculated by formula ,

$Vf = (M \upsilon/k\eta)^{3/2} \ m^3$

Where, M is the molecular weight

'k' is a temperature independent constant equal to 4.28×10^9 for all liquids.

4. Acoustic impedance (Z): The acoustic impedance is computed by the formula

$Z = \upsilon \times \rho \ kg \ m^{-2} s^{-1}$

5. Free length (Lf): It is calculated on using formula,

$L_f = (K\sqrt{\kappa})$

κ =Adiabatic compressibility,.K=Temperature dependent constant(93.875+0.345T)x10^{-8}

6. Attenuation (α/f^2): It is calculated by,

$\alpha/f^2 = 8\pi^2\eta/3\rho\upsilon^3$

7. Viscous relaxation time (Ʈ): It is calculated by using the relation,

$Ʈ = 4\eta/3\rho\upsilon^2$

8. Rao's Constant (R): Rao's constant is calculated by using formula,

$R = V \, . \upsilon^{\frac{1}{3}}$ or $R = \left(\frac{M}{\rho}\right)\upsilon^{\frac{1}{3}}$

M= Molecular Weight.

9.Wada constant (W): It was calculated by formula,

$W = M.\ \kappa^{-1/7}/\rho$

10. Internal pressure(Πi): On using below cited formula Internal pressure is calculated,

$$\Pi i = bRT\left[\frac{k\eta}{v}\right]^{1/2} \frac{\rho^{\frac{2}{3}}}{M^{\frac{7}{6}}}$$

11.Molar volume: It is the ratio of density & molecular weight

$$Vm = \frac{M}{\rho}$$

12.Cohesive energy (CE) **:** Cohesive energy is calculated by formula quoted below,

$$CE = \Pi i Vm$$

Result and Discussion

The measured values of ultrasonic velocity, density and related thermo acoustical parameters of chloroquine phosphatewith water at 318K temperatures in different

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concentrations temperatures in different concentrations are shown in table1 and 2 .The variation of acoustical parameters with concentrations and temperature is shown graphically in fig.1 to 14.

Table 1:- Ultrasonic velocity, Density, Viscosity, Adiabatic compressibility, Intermolecular free length, Free volume , Rao's constant of different % concentration of solution of compounds in water at ,318 K

Solution of chloroquine phosphate in water at 318 K

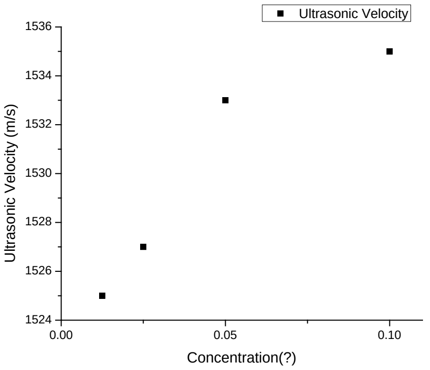
Concentration(%)	Density (Kgm^{-3})	Viscosity x10^{-3} (Nsm	Ultrasonic Velocity (m/s)	Adiabatic compressibility x10^{-10} (m^2 /N)	Intermolecular free length x10^{-11} (m)	Free Volume x10^{-3} (m^3 mol	Rao's constant
0.0125	997.52	0.7913	1525	4.311	4.1195	111.91	5.9525
0.025	998.96	0.8192	1527	4.293	4.1109	106.45	5.9465
0.05	1000.16	0.8481	1533	4.254	4.0922	101.65	5.9471
0.1	1004.44	0.9173	1535	4.225	4.0782	90.54	5.9243

Table. 2- Internal pressure, Acoustic impedence, Relaxation time, ultrasonic attenuation, cohessive energy and molar volume,Wada's constant, Rao's constant at 318 K

Solutin of Chloroquine phosphate in water at 318 K

Concentration(%)	Internal pressure x10^3(Nm^{-2})	Acoustic Impedence x 10^6 (Kg^{-1} m^2 S^{-1}	Relaxation time (S)x10^6	Attenuation x10^{-15} (s^2m^{-1})	Rao's Constant(R)	Wada's constant x10^1	Cohessive energy x10^3 (KJ/Mol)	Molar volume x10-3 (m^3/mol)
0.0125	16.227	1.521	2.4476	5.892	5.9525	1.1259	8.3911	517.1
0.025	16.516	1.525	2.5442	6.067	5.9465	1.1250	8.5289	516.4
0.05	16.785	1.533	2.6579	6.200	5.9471	1.1253	8.6579	515.8
0.1	17.495	1.542	2.8946	6.651	5.9243	1.1214	8.9855	513.6

The following figures shows the variation of various acoustical parameters with concentration and temperature.



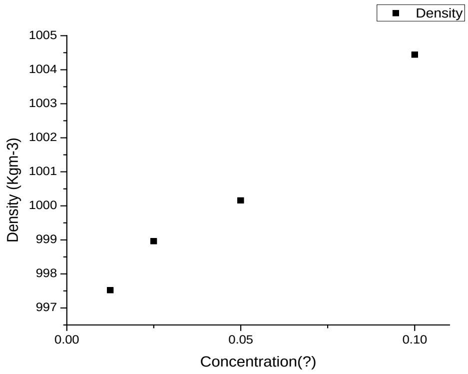


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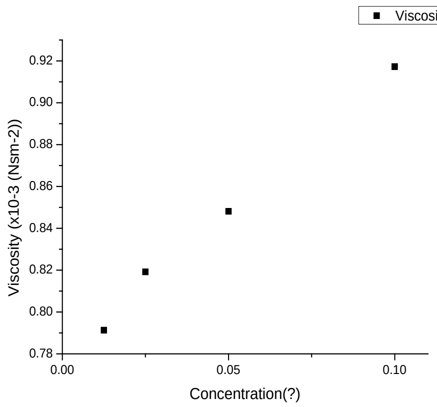
Figure:1-variation of ultrasonic velocity with concentration

Figure:2-variation of density withconcentration



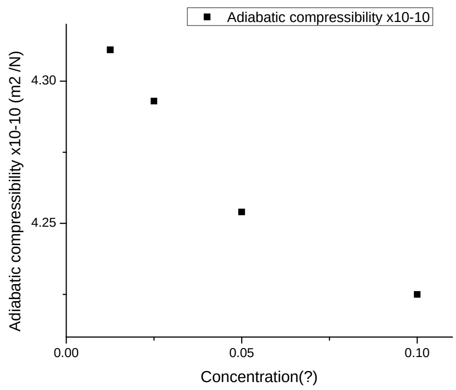
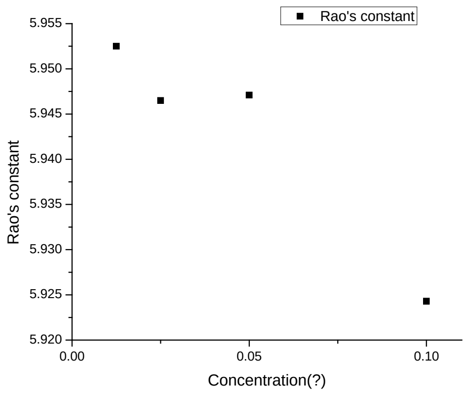


Figure:3-varation of viscosity with concentration with concentration

Figure:4-varation of adiabatic compressibility



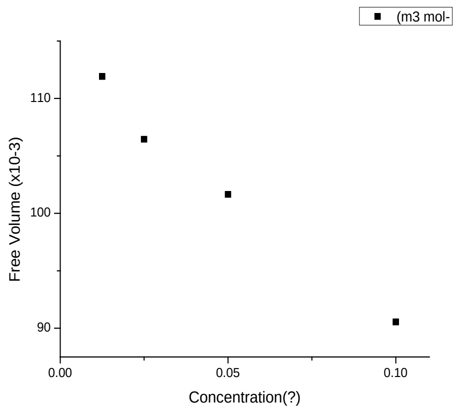


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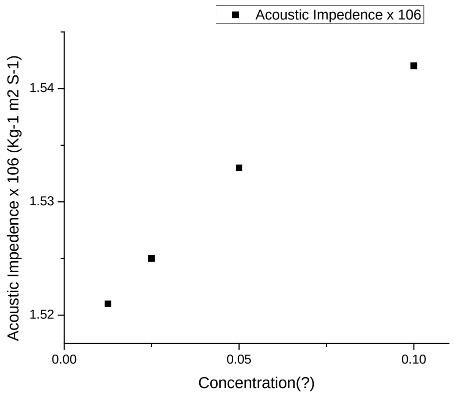
Figure:5-varation of Rao's constant with concentration concentration

Figure:6-varation of free volume with



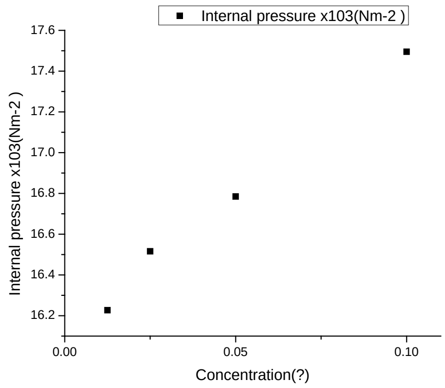


Figure:7-varation of acoustic impedence concentrationwith concentration

Figure:8-varation of acoustic internal pressurewith

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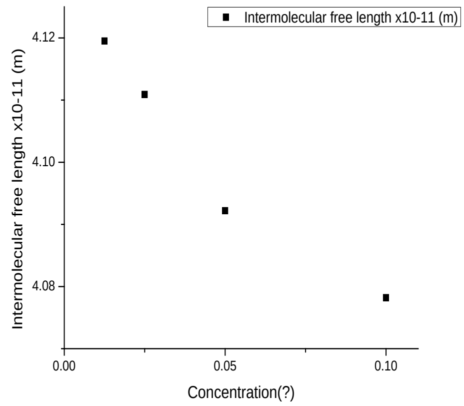


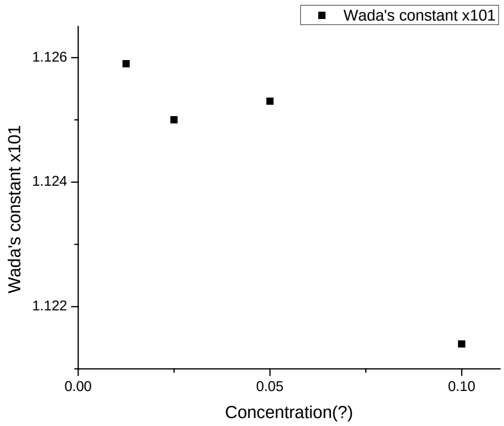
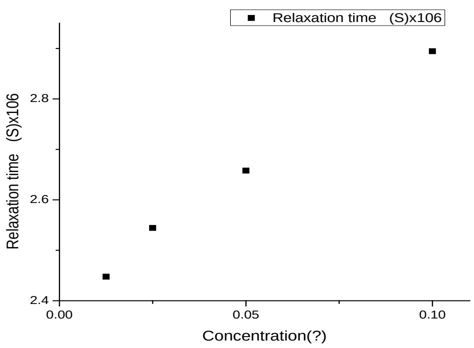


Figure:9-varation of intermolecular free Figure:10-varation of Wada’s constant
length with concentration with concentration



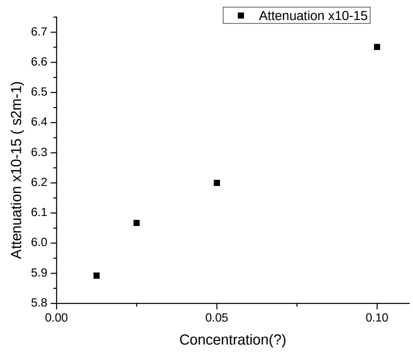
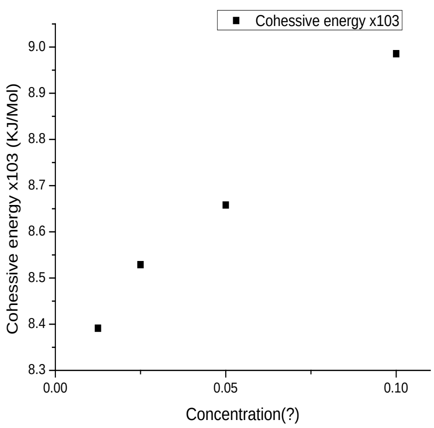


Figure:11-varation of relaxation time withFigure:12-varation of ultrasonic attenuation
concentration with concentration



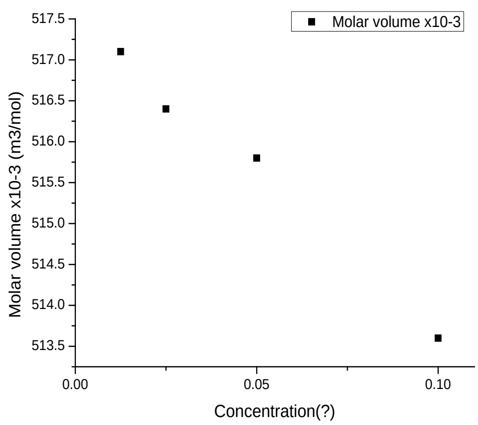


Figure:13-varation of cohessive energy Figure:14-varation of molar volume with
with concentration concentration

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It is observed that ultrasonic velocity and acoustic impedance shows nonlinear increasing variation with increase in molar concentration. This indicates the complex formation and intermolecular weak association which may be due to hydrogen bonding. Thus complex formation can occurs at these molar concentrations between the component molecules. Adiabatic compressibility (βa) shows an inverse behavior compared to the ultrasonic velocity. Adiabatic compressibility decreases with increase in concentration of chloroquine phosphate. The decrease in compressibility implies that there is an enhanced molecular association in the system with increase in solute concentration.

The opposite trend of ultrasonic velocity and adiabatic compressibility indicate association among interacting chloroquine phosphate and water molecules. In the present system of aqueous chloroquine phosphate free length varies nonlinearly with increase in molar concentration which suggests the significant interaction between solute and solvent due to which structural arrangement is also affected.

Relaxation time decreases with increase in concentration. Nonlinear trend of density with concentration indicates the structure-making and breaking property of solvent due to the formation and weakening of H-bonds. The free volume increases and internal pressure decreases with increases in molar concentration indicate the association through hydrogen bonding. It shows the increasing magnitude of interaction between the chloroquine phosphate and water.

Conclusion

The acoustical parameters suggest the strong molecular interaction in the solution. Ultrasonic study of aqueous solution of chloroquine phosphate at different concentrations give most useful information in understanding interaction of solute with solvent.In the present paper the ultrasonic velocity (υ),density and acoustical parametersadiabatic compressibility (βa), relaxation time (τ), acoustic impedance (z), free length (Lf), free volume (Vf) and internal pressure (Pi),Wada's constant(W), Rao's constant (R) have been measured at different concentrations. The parameters indicate that there is a strong molecular interaction.

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