

# Ultrasonic Behaviour of Chloroquine in Aqueous Solution of Acetic Acid at 298.15K

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**Abstract:** The densities, ultrasonic velocity ( $U$ ), adiabatic compressibility ( $\beta$ ), Acoustic impedance ( $Z$ ), Intermolecular free length ( $L_f$ ) and apparent molar compressibility ( $K_\phi$ ) of chloroquine in water and aqueous solution of acetic acid at 298.15K were calculated. From density and ultrasonic data the values of ultrasonic parameters had been determined which are correlated and discussed in terms of molecular interactions present in the system.

**Keywords:** adiabatic compressibility, apparent molar compressibility, intermolecular free length, acoustic impedance, ion-solvent interaction.

## 1. Introduction

Physicochemical properties provide detailed information regarding structural changes in aqueous electrolytic solutions and are highly affected by solvents. These properties are explained in terms of ion-solvent and solvent-solvent interaction which helps to understand the structure making and breaking properties of solutes<sup>1</sup> using ultrasound in different fields.<sup>2-5</sup> So derived ultrasonic parameters are being extensively used to study the molecular interactions in pure liquids<sup>6-8</sup>, liquid mixtures<sup>9-11</sup> and electrolytic solutions<sup>12</sup>. The effect on concentration of solute and volume of solvent on acoustic/ultrasonic parameters like ultrasonic velocity ( $U$ ), adiabatic compressibility ( $\beta$ ), apparent molar compressibility ( $K_\phi$ ) etc have been investigated which give important information about the intermolecular forces in determining the properties of mixture<sup>13</sup>. The ultrasonic velocity and its related parameters of chloroquine in aquo-organic solutions have been derived. The drug chloroquine is used as antiviral agent against chikungunya fever and extensively used in the treatment and prevention of malaria<sup>14-16</sup>. It is also used in some autoimmune disorders such as rheumatoid arthritis. This present work aims at physico-chemical studies involving determination of ultrasonic properties of chloroquine in aqueous solution of acetic acid at 298.15K.

## 2. Material and methods

In this investigation the following chemicals were used: chloroquine, acetic acid and distilled water. Chloroquine was obtained from a local pharmaceutical company. Water used in this study was double distilled water prepared by distilling water over alkaline potassium permanganate in all glass distillation flasks. Acetic acid used for the study was Anal R grade. All solutions were prepared in concentrations from 0.002-0.01M. The ultrasonic velocity was measured by single crystal interferometer (Mittal, model-81) operating at a frequency of 2MHz. The temperature was maintained constant at 298.15K in a thermostat. The density of solutions was determined accurately using specific gravity bottle and electronic balance of accuracy ( $\pm 0.1$  mg).

## 3. Theory

All the binary aqueous mixtures of acetic acid were prepared by v/V ratio in terms of mole fraction and the solutions of chloroquine were made by weight and the conversion of molality (m) into molar concentration (c) was done by using the standard expression,

$$C = md(1 + 0.001mM_2)^{-1} \quad (1)$$

The adiabatic compressibility ( $\beta$ ) is a measure with which a system can be compressed. This parameter determines the physico-chemical properties of mixtures.

The values of  $\beta$  calculated for solutions of different concentrations is of the form,

$$\beta = d^{-1}U^{-2} \quad (2)$$

Acoustic impedance ( $Z$ ) is defined as

$$Z = Ud \quad (3)$$

Intermolecular free length ( $L_f$ ) can be determined by the equation,

$$L_f = K_j \beta^{1/2} \quad (4)$$

where  $K_j$  is Jacobson constant =  $2.0965 \times 10^{-6}$

The apparent molar properties are found to depend on the concentration of solutions. The apparent molar compressibility,  $K_\phi$  can be computed from the equation<sup>17</sup>,

$$K_\phi = 1000\beta c^{-1} - \beta^0 d^{-1}(1000c^{-1} - M_2) \quad (5)$$

where  $\beta^0$  is the adiabatic compressibility of the solvent

## 4. Result and Discussion

The experimental densities, ultrasonic velocity ( $U$ ), adiabatic compressibility ( $\beta$ ), Acoustic impedance ( $Z$ ), Intermolecular free length ( $L_f$ ), apparent molar compressibility ( $K_\phi$ ) of chloroquine in water and aqueous solution of acetic acid at 298.15K in Table-1 are shown.

Table 1

Mole Fraction ( $X_{org}$ )	Concentration ( $c$ ) mol dm <sup>-3</sup>	Density ( $d$ ) $\times 10^3$ (kgm <sup>-3</sup> )	Ultrasonic velocity ( $U$ ) msec <sup>-1</sup>	Adiabatic compressibility ( $\beta$ ) $\times 10^{-7}$ m <sup>2</sup> N <sup>-1</sup>	Acoustic Impedance ( $Z$ ) $\times 10^{-3}$ kg m <sup>2</sup> s <sup>-1</sup>	Intermolecular free length ( $L_f$ ) $\times 10^{-7}$ m	Apparent molar compressibility $- (K_\phi) \times 10^{-5}$ m <sup>2</sup> N <sup>-1</sup>
Chloroquine in water							
	0.002M	0.9953	1510.2	4.4053	1.5031	1.3915	-3.6643
	0.004M	1.0008	1516.3	4.3459	1.5175	1.3821	1.8106
	0.006M	1.0011	1525.5	4.2924	1.5272	1.3736	1.3491
	0.008M	1.0046	1528.9	4.2584	1.5359	1.3681	1.0292
	0.01M	1.0063	1533.2	4.2274	1.6032	1.3631	0.8416
Chloroquine in acetic acid-water							
0.073	0.002M	1.0181	1556.8	4.0527	1.5849	1.3346	4.8520
	0.004M	1.0170	1558.0	4.0508	1.5844	1.3343	2.4363
	0.006M	1.0159	1561.3	4.0381	1.5861	1.3322	1.6490
	0.008M	1.0185	1562.8	4.0201	1.5917	1.3293	1.2392
	0.01M	1.0183	1564.9	4.0106	1.5934	1.3277	0.9987
0.174	0.002M	1.0351	1590.2	3.8204	1.6461	1.2958	5.6090
	0.004M	1.0421	1598.2	3.7541	1.6561	1.2845	2.8754
	0.006M	1.0364	1602.0	3.7597	1.6603	1.2854	1.9473
	0.008M	1.0356	1604.1	3.7527	1.6612	1.2843	1.4701
	0.01M	1.0369	1606.2	3.7354	1.6623	1.2813	1.1840
0.321	0.002M	1.0486	1629.3	3.5924	1.7085	1.2566	6.7410
	0.004M	1.0498	1633.1	3.5721	1.7143	1.2530	3.1724
	0.006M	1.0500	1634.5	3.5648	1.7162	1.2517	2.1452
	0.008M	1.0493	1635.3	3.5633	1.7161	1.2514	1.6177
	0.01M	1.0506	1639.7	3.5433	1.7219	1.2480	1.3050
0.558	0.002M	1.0828	1659.2	3.3569	1.7954	1.2125	6.8119
	0.004M	1.2015	1662.4	3.0117	1.9974	1.1923	3.0897
	0.006M	1.2181	1664.4	2.9635	2.0274	1.1627	2.5392
	0.008M	1.2482	1667.3	2.8820	2.0811	1.1564	1.5018
	0.01M	1.2951	1669.1	2.7716	2.1617	1.1385	1.1614

It is evident from Table 1 that the values of density increase with concentration. It is due to increase in hydrophilic interaction. The increase in density relates to shrinkage in the volume which in turn due to the presence of solute molecules. The ultrasonic velocity also increases with increase in concentration of chloroquine and molefraction of acetic acid. But for acetic acid-water it is higher than that of water system. The adiabatic compressibility decreases for both water and acetic acid-water system. These values are much lower for chloroquine in acetic acid-water system. The difference in  $\beta$ s may be accounted to solvation behaviour. The decrease in  $\beta$  values with increasing concentration of solute might be due to aggregation of acetic acid solvent molecules around chloroquine. In other words a bounded solvation layer around chloroquine leads to decrease in  $\beta$  values. Acoustic impedance ( $Z$ ) is a measure of characteristic of the medium offered by infinite media for propagation of sound through it. The values of  $Z$  increase for both the systems. But higher impedance for chloroquine in acetic acid-water system indicates ion-solvent or solvent-solvent interactions due to the presence of bulkier solvated ion. The intermolecular frelength depends upon the intermolecular attractive or repulsive forces. In the present investigation  $L_f$  values are found to decrease with increase in concentration of chloroquine indicating significant molecular association between chloroquine and acetic acid molecule suggesting a structure promoting behavior on addition of solute. The variation of  $K_\phi$  with concentration

for water and acetic acid-water system are shown by Figure 1 and 2 respectively.

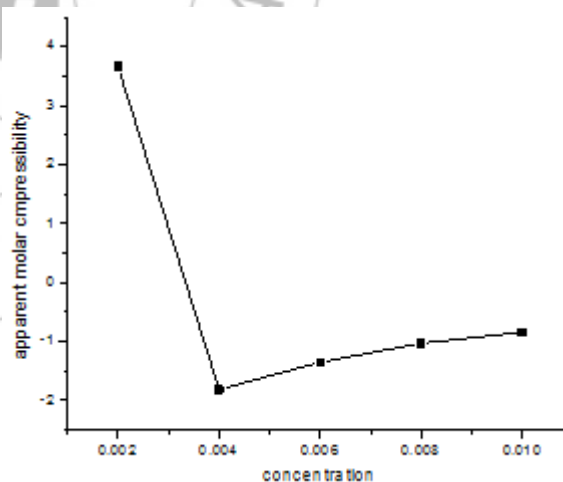
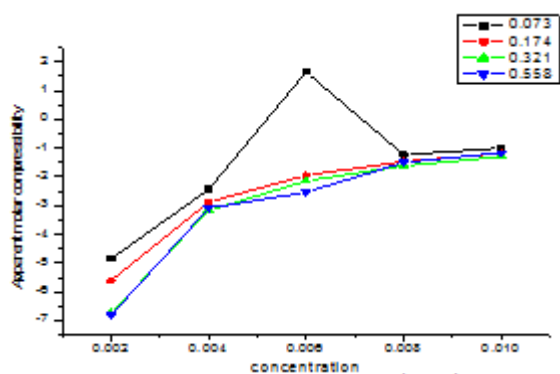


Figure 1: Variation of apparent molar compressibility ( $K_\phi$ ) with  $c$  for chloroquine in water at 298.15K



**Figure 2:** Variation of apparent molar compressibility ( $K_{\phi}$ ) with  $c$  for chloroquine in different mole fraction of acetic acid at 298.15K

The negative values of  $K_{\phi}$  indicate ionic, dipolar and hydrophilic interactions occurring in these systems. More number of solvent molecules available at lower concentration of acetic acid favors the penetration of chloroquine into solvent molecules. So larger negative  $K_{\phi}$  value of chloroquine in acetic acid-water possesses strong ion-solvent interaction as compared to water system.

## 5. Conclusion

The ultrasonic data suggest that solvent-solvent interactions result at higher mole fraction of acetic acid because of the formation of hydrogen bonding with water. But at low mole fraction of acetic acid, ion-solvent interaction predominates over solvent-solvent interaction. From the observed parameters it has been concluded that in aqua-organic solutions ion-solvent interaction is much stronger for chloroquine as compared to its aqueous solution.

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