Molecular interaction studies on pharmaceutical drug of 2-[1-(aminomethyl) cyclohexyl] acetic acid in water of various concentrations at 303K

S. Rajesh and V. Balasubramanian

Department of Chemistry, AMET University, Chennai, Tamilnadu, India

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ABSTRACT

The measurement of ultrasonic velocity in pure liquids and mixtures is an important tool to study the physico- chemical properties and also explains the nature of molecular interactions. The study of thermodynamic parameters to explain molecular interaction of drugs in aqueous or non- aqueous medium provides useful information in medicinal and pharmaceutical chemistry. In present work molecular interaction of aqueous solution of 2-[1-(aminomethyl) cyclohexyl] acetic acid at different concentrations at 303K was studied by measuring ultrasonic velocity, density and viscosity of the solution. The ultrasonic parameters such as adiabatic compressibility, free volume, free length, acoustic impedance, absorption coefficient, viscous relaxation time, available volume and Lenard Jones Potential were calculated. These parameters explained formation of hydrogen bond and molecular interaction existing in the solution.

Keywords: Hydrogen bond, Free volume, Free length, Ultrasonic velocity, Molecular interaction.

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INTRODUCTION

The rapid development of ultrasonic techniques for producing powerful ultrasonic vibrations have opened up wide fields of research and technical applications in physics, chemistry, biology, medicine and industry. Ultrasonic is an area of intense scientific and technological research. Science and technology of ultrasonic is widely sought in the recent years for industrial and medicinal application. The literature survey on acoustical studies of solutions reveals that ultrasonic measurements are used to estimate the different elastic properties of the molecule from which the type of molecular interactions can be very well understood [1-4]. The measurement of ultrasonic velocity in pure liquids and mixtures is an important tool to study the physico- chemical properties and also explains the nature of molecular interactions [5-7].

In the present investigation we tried to study molecular interaction of aqueous 2-[1-(aminomethyl) cyclohexyl] acetic acid solution by measuring ultrasonic velocity, density and viscosity for various concentrations at 303K. From the data acoustic parameters such as adiabatic compressibility, free volume, free length, acoustic impedance, absorption coefficient, viscous relaxation time, available volume and Lenard Jones Potential were calculated. Effect of concentration on molecular interaction is studied from acoustic and thermodynamic parameters.

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EXPERIMENTAL SECTION

The chemicals used were of analytical grade. Double distilled water was used for preparation of solutions. 2-[1-(aminomethyl) cyclohexyl] acetic acid was dissolved in water of various ratio's to prepare different concentration 0.2%, 0.4%, 0.6%, 0.8% and 1.0%. The binary mixture are prepared by using volume percentage(%) by using jobs variation method [8-10]. The ultrasonic velocities of aqueous solutions were measured using ultrasonic interferometer (model F05) supplied by Mittal Enterprises, New Delhi operating at the frequency of 2MHZ with the accuracy of ± 0.01 ms-1. The densities(ρ) of solutions were determined using specific gravity bottles of capacity 10ml. The viscosities(η) of the solutions are measured using Oswald's viscometer. The temperature was maintained at $303 \pm 0.1K$ during the measurement of ultrasonic velocity, density, and viscosity values. The acoustical parameters are calculated from U, ρ, and η [11-14] using following relation.

1. Ultrasonic Velocity (U)
The relation used to determine the ultrasonic velocity is given by,

$$U = f\lambda \text{ ms}^{-1}$$

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

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

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

Where,
U – Ultrasonic velocity
ρ – Density of the solution.

3. Free Volume (V_f)
Free volume in terms of the ultrasonic velocity (U) and the viscosity of the liquid (η) as $V_f = (M_{eff}U/k\eta)^{3/2} \text{ m}^3$

Where, M_{eff} is the effective molecular weight ($M_{eff} = \Sigma$ mi xi, in which mi and xi are the molecular weight and the mole fraction of the individual constituents respectively and 'k' is a temperature independent constan t equal to 4.28×10^9 for all liquids.

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

$$Z = U\rho \text{ kgm}^{-2}\text{s}^{-1}$$

Where
U –Ultrasonic velocity
ρ –Density of the solution

5. Free Length (L_f)
Jacobson [15] introduced the concept of the free length in liquids. He suggested the following relation to calculate the intermolecular free length.

$$L_f = (K/U \rho^{1/2}) \text{ m}$$

Where
U - Ultrasonic velocity of liquid

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ρ - Density of liquid
K - Jacobson temperature dependent constant defined as

K = (93.875 + 0.345T) X 10^{-8}

6. Absorption Coefficient (α/f^2)
The absorption coefficient (α/f^2), also sometimes called attenuation coefficient. It is defined as

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

7. Available Volume (V$_a$)
The available volume (V$_a$) is a direct measure of compactness and the strength of bonding between the molecules of a liquid or liquid mixture. It can be calculated from following relation

$$V_a = V_m(1- U/U_a)\ m^3$$

Where V$_m$ is the molar volume and U$_a$=1600ms^{-1}

8. Lenard Jones Potential (LJP)
The Lenard Jones potential exponent is given by [16]

$$LJP = 6V_m/V_a$$

Where
V$_m$ - the molar volume   V$_a$ - the available volume

9. Viscous Relaxation time (τ)
Relaxation time (τ) and absorption coefficient are directly correlated. The absorption of a sound wave is the result of the time lag between the passing of the ultrasonic wave and the return of the molecules to their equilibrium position. It is calculated using the relation [17],

$$\tau=4\eta/3\rho U^2$$

Where
η - viscosity of the solution
ρ - density of solution
U - ultrasonic velocity of the solution

RESULTS AND DISCUSSION

The measured ultrasonic velocities (U), densities (ρ), viscosities (η) and other acoustical parameters such as adiabatic compressibility (κ), free volume (V$_f$), free length (L$_f$), acoustic impedance (Z), absorption coefficient (α/f^2), viscous relaxation time (τ), available volume (V$_a$), Lenard jones potential (LJP) values at 303K is given in the tables 1 & 2.

Table 1. Ultrasonic velocity (U), Density (ρ), Viscosity (η), Adiabatic Compressibility (κ), Free Volume (V$_a$), and Acoustic Impedance (Z) of 2-[1-(aminomethyl) cyclohexyl] acetic acid + Water system at various Concentrations
[Temp: 303K]

Conc. %	U/ms^{-1}	ρ/ kgm^{-3}	$\eta/10^{-4}$ Nsm^{-2}	$\kappa/10^{-10}$ kg^{-1} ms^{-2}	V$_f/10^{-4}$ m^3	Z/10^5 kgm^{-1}s^{-1}
0.2	1520	1093.20	8.336	3.95	6.805	1.66
0.4	1518	1091.20	8.341	3.97	6.886	1.65
0.6	1510	1095.60	8.674	4.00	6.537	1.65
0.8	1500	1094.40	8.817	4.06	6.408	1.64
1.0	1497	1094.80	8.892	4.07	6.404	1.63

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Table 2. Free Length (L_f), Absorption Coefficient (α/f^2), Available Volume (V_a), Lenard Jones Potential (LJP), and Viscous Relaxation time (τ) of 2-[1-(aminomethyl) cyclohexyl] acetic acid + Water system at various Concentrations

[Temp: 303K]

Conc. %	L_f/ 10^{-11} m	α/f^2/10^{-11} Npm^{-1}s^{-1}	V_a/10-4 m3	LJP	τ/10^{-9}
0.2	3.947	5.70	8.30	115.60	4.40
0.4	3.956	5.74	8.61	117.07	4.42
0.6	3.969	6.04	9.50	106.73	4.62
0.8	3.998	6.27	10.62	96.04	4.77
1.0	4.005	6.36	11.11	93.21	4.83
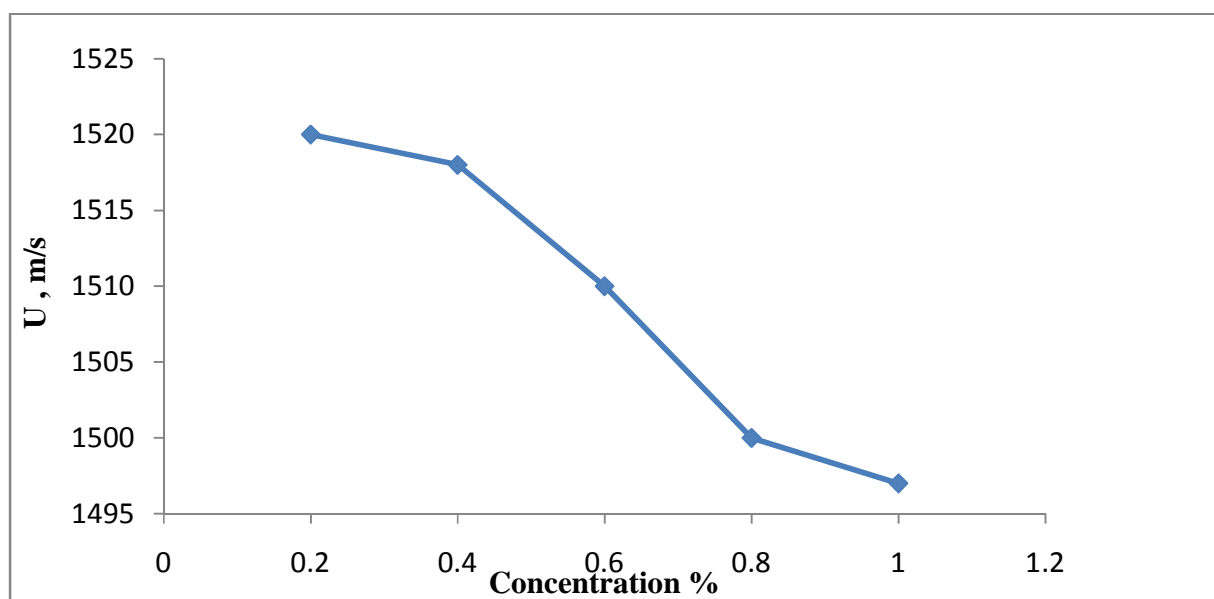
Fig. 1. Plot of ultrasonic velocity versus concentration
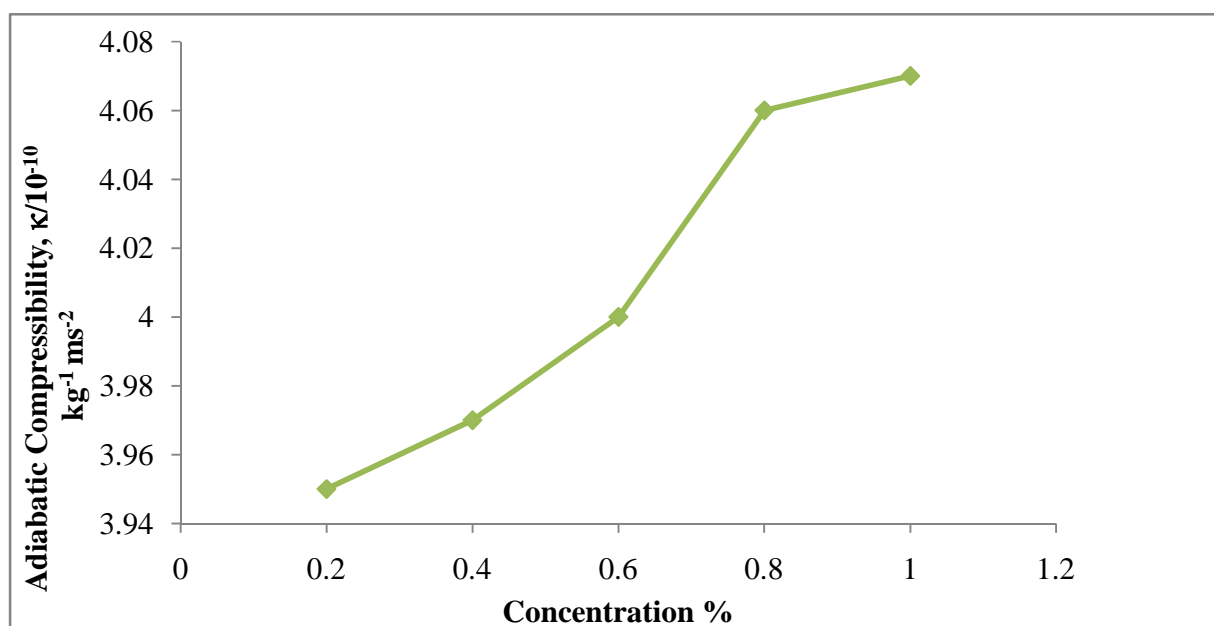
Fig. 2. Plot of adiabatic compressibility versus concentration.
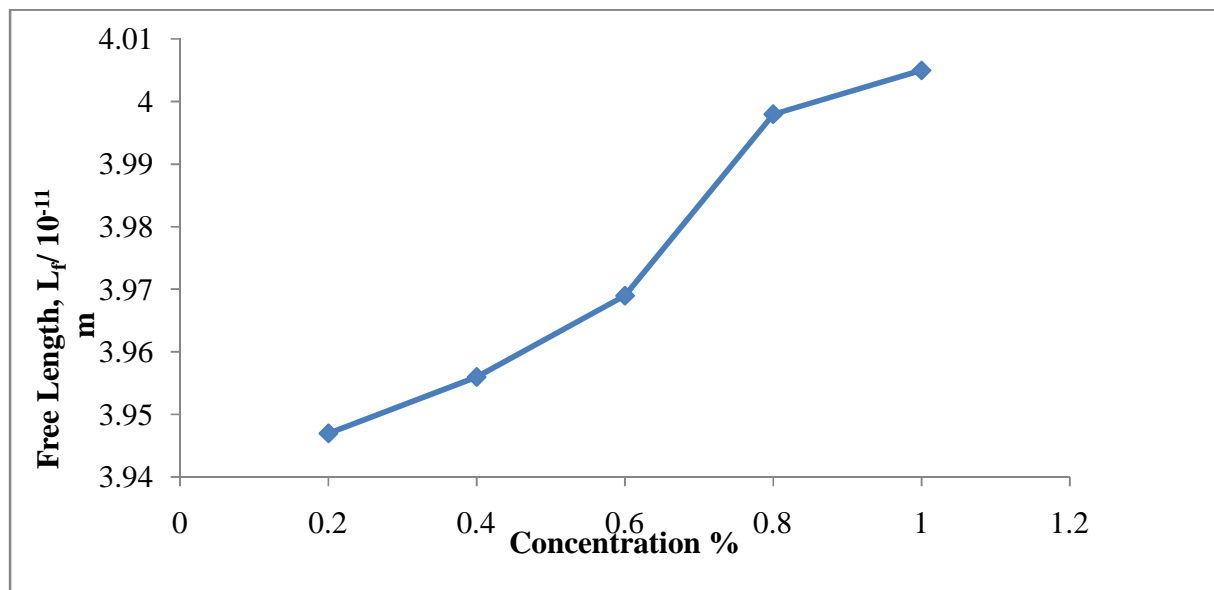
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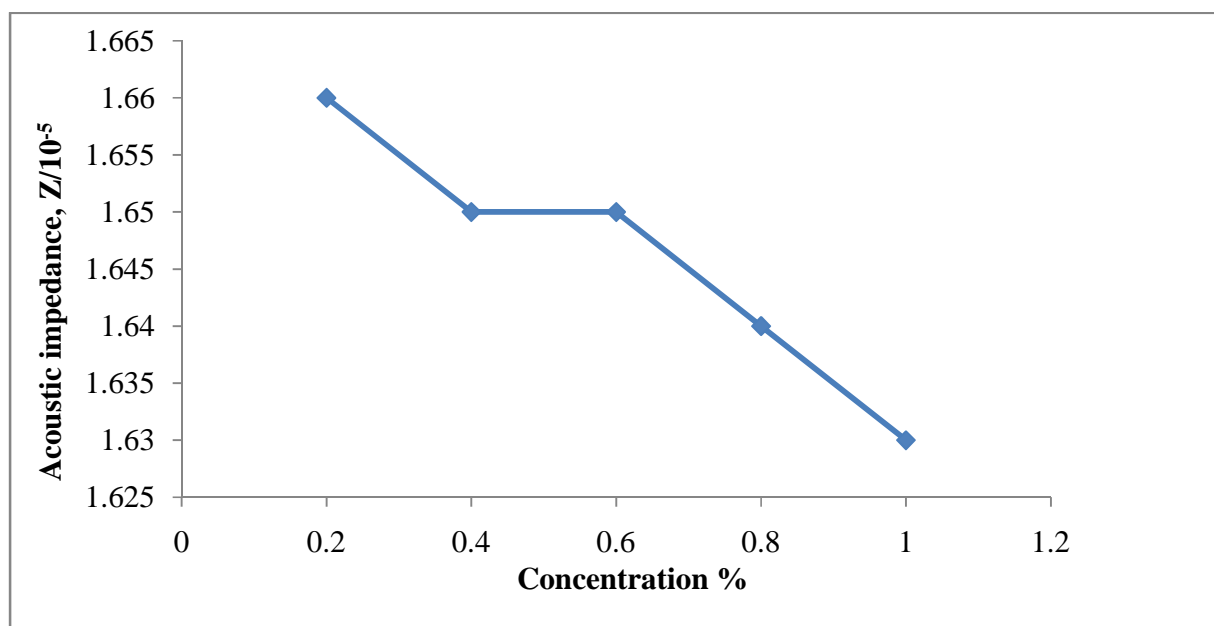

Fig. 3. Plot of free length versus concentration

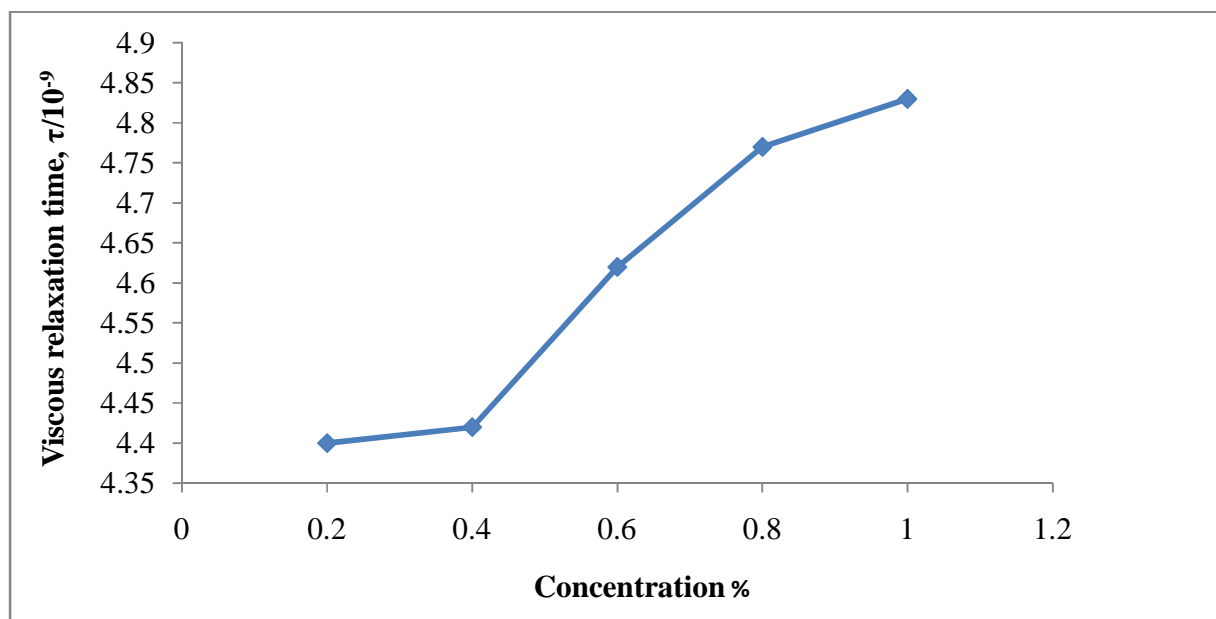Fig. 4. Plot of acoustic impedance versus concentration

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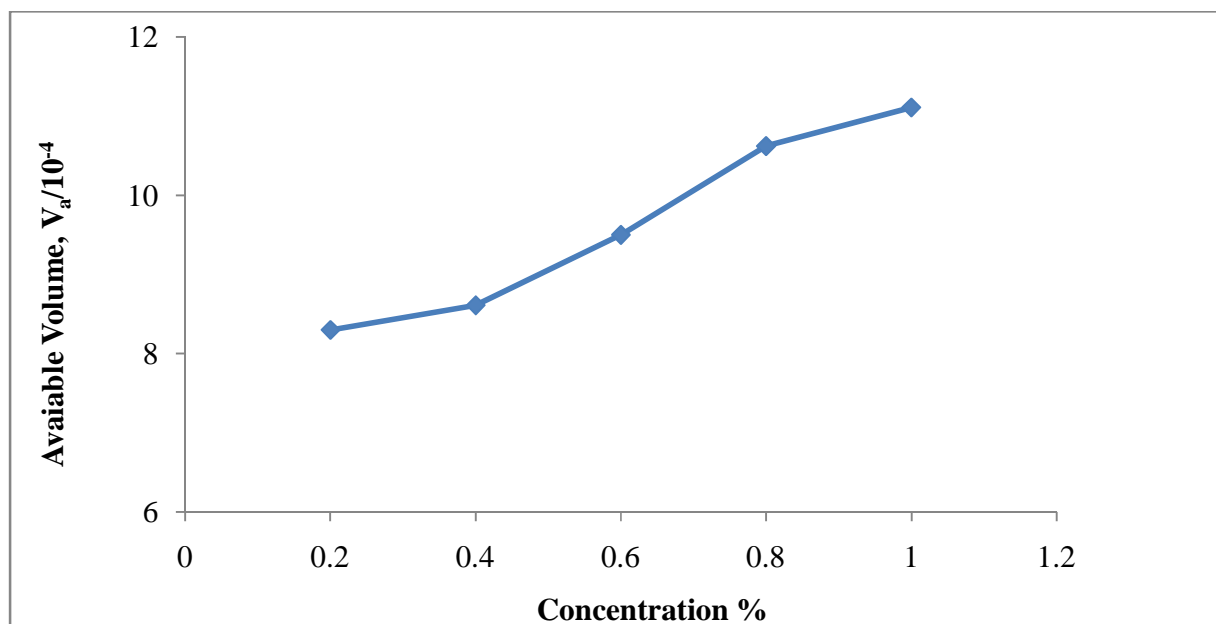**Fig. 5. Plot of viscous relaxation time versus concentration**

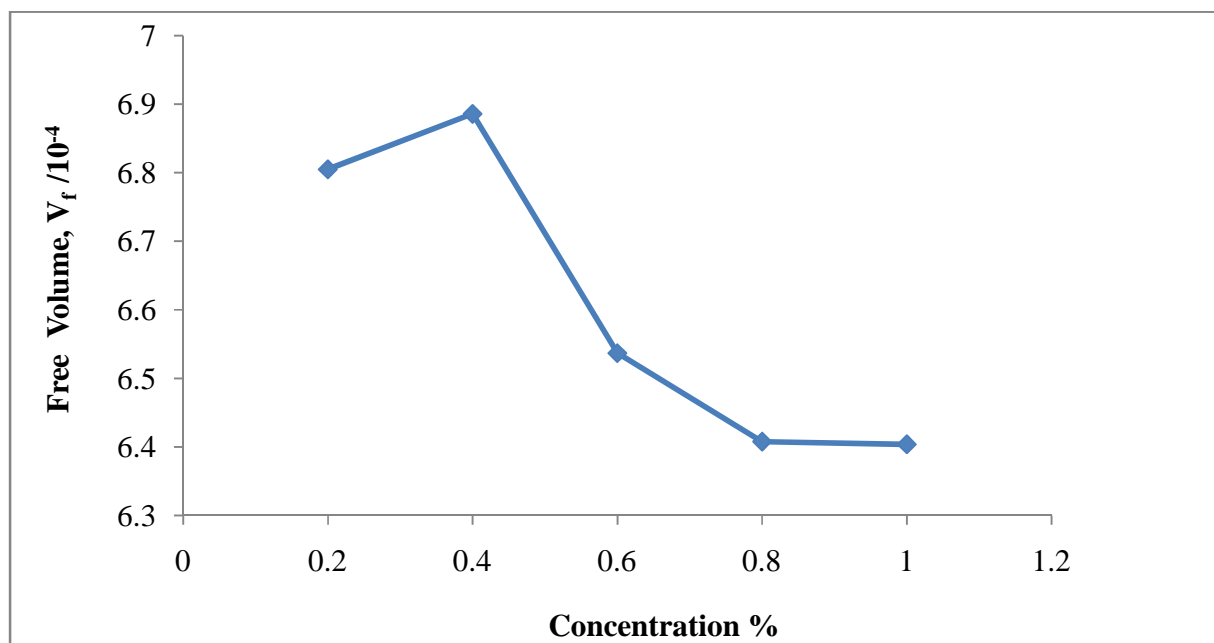**Fig. 6. Plot of available volume versus concentration**

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Fig. 7. Plot of free volume versus concentration

From the tables 1 & 2 it is noted that the density and viscosity increases with increase concentration of the solution. Ultrasonic velocity in a liquid system depends on the structure and molecular properties. Ultrasonic velocity decreases with increase concentration of the system. The decrease in velocity is due to the increase in free length and adiabatic compressibility of the liquid mixture. This may lead to the presence of specific molecular interaction between the molecules of the liquid mixture. The adiabatic compressibility and free length are the deciding factors of the ultrasonic velocity in liquid system.

Intermolecular free length increases with increase concentration of the present system. This indicates that the distance between surfaces of molecules increases, thereby reducing the ordering of molecules. According to the observation of Tabhane and Patki [18], an increase in the adiabatic compressibility shows a tendency towards less ordering resulting in a decrease of ultrasonic velocity with volume percentage of one component. Thus the variation of intermolecular free length and adiabatic compressibility suggests that molecular arrangement becomes less ordered.

Fig. 2 & 4 shows the specific acoustic impedance and adiabatic compressibility exhibit opposite trend. From fig. 7 the decrease in free volume shows that the strength of interaction decreases gradually with the increase in solute concentration. It represents that there is weak interaction between the solute and solvent molecules.

The relaxation time (τ) increase with increasing concentration of the system. The dispersion of the ultrasonic velocity in the system should contain information about the characteristic time τ of the relaxation process that causes dispersion. The relaxation time which is in the order of 10^{-12} sec is due to structural relaxation process [19] and in such a situation it is suggested that the molecules get rearranged due to co-operative process [20]. Acoustic impedance decreases with increase the concentration of the system.

CONCLUSION

The computed acoustical parameters and their values point to the presence of specific molecular interaction in the mixture. Hence it is concluded that the association in the mixture is the result of intermolecular Hydrogen bonding in Binary liquid mixture.

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