



## ULTRASONIC INVESTIGATION OF MOLECULAR INTERACTIONS IN BINARY LIQUID MIXTURES AT 298 K AND 2 MHZ FREQUENCY

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Communicated : 23.01.2023

Revision : 28.02.2023 & 08.03.2023

Accepted : 03.04.2023

Published : 30.05.2023

### ABSTRACT:

Ultrasonic studies may throw more light on the molecular interaction to know the behaviour of solute and solvent molecules in liquid mixtures and solutions. Measurements of ultrasonic velocity, density and viscosity have been carried out for 1-Heptanol in Acrylonitrile at different concentrations at 298 K temperature and 2 MHz frequency, to provide information about molecular environment and extent of molecular interaction by ultrasonic technique. Ultrasonic velocity study of binary liquid mixture has gained much importance in assessing the weak and strong molecular interactions and association between the component molecules. Acoustical parameters such as adiabatic compressibility ( $\beta_a$ ), intermolecular free length ( $L_f$ ), Acoustic Impedance ( $Z$ ) and Relaxation time ( $\tau$ ) for n- Heptanol in Acrylonitrile were calculated from ultrasonic velocity and effect of concentration on molecular interaction was predicted.

**Keywords :-** Acrylonitrile, concentration, n- Heptanol, molecular, ultrasonic.

### INTRODUCTION :

In recent years, understanding the nature of molecular interactions necessitates a study of liquids and liquid mixtures using ultrasonic technology. Thermo-acoustic properties of liquid mixtures have been widely used to investigate the departure of actual liquid mixture behaviour from ideality. The calculated acoustical parameters and ultrasonic velocity reveal important information about molecular interactions. Through ultrasonic investigation of liquid mixtures containing polar and non-polar components, it is possible to gain an understanding of the molecular interactions and structural behaviours of molecules and their mixtures. Intermolecular interactions influence both the structural arrangement and the shape of molecules [1-3]. At different temperatures, ultrasonic velocities, as well as density and viscosity, are measured at 298K temperature to gain a better understanding of the physicochemical properties and molecular

interactions between the contributing components of these mixes. In most of the solutions, ultrasonic velocity is a temperature-dependent quantity. It is also affected by the solute concentration. Density, viscosity, and other thermodynamic parameters are measured and used to explain the nature, strength, and order of the molecular interaction. Spectroscopic methods can be used to investigate molecular interactions [4-6]. The ultrasonic technique is widely used over these methods because it is less expensive, easier to use, takes less time, and produces more precise results. An attempt has been made in this work to examine the variety of thermodynamic properties of aqueous [5-7]. From graphical and analytic perspectives, the nature of the mixture is varied in temperature, size, shape, and nature in order to understand its nature.

In present work the accurate thermodynamic and acoustic properties of higher alcohol particularly 1-Heptanol and Acrylonitrile have

been calculated at 298K. The acoustic parameters are used to explain interaction in this binary mixture.

#### **MATERIALS AND METHODS :**

The ultrasonic velocity (U) in binary liquid mixtures for 1- Heptanol in acrylonitrile been measured using an ultrasonic interferometer (Mittal type, Model F-81) working at 2 MHz frequency and at temperature 298 K. The accuracy of sound velocity was  $\pm 0.1 \text{ ms}^{-1}$ . An electronically digital operated constant temperature water bath has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desire temperature. The density of pure liquids and liquid mixtures was determined using pycnometer by relative measurement method with an accuracy of  $\pm 0.1 \text{ Kg m}^{-3}$ . All the precautions were taken to minimize the possible experimental error.

The parameters such as adiabatic compressibility ( $\beta_a$ ), intermolecular free length ( $L_f$ ), Acoustic Impedance (Z) and relaxation time ( $\tau$ ) are calculated by using the following relation (1- 4).

$$\beta_a = (U^2 \rho)^{-1} \quad \dots (1)$$

$$L_f = KT\beta_a^{-1/2} \quad \dots (2)$$

$$Z = U\rho \quad \dots (3)$$

$$\tau = 4/3 \eta \beta_a \quad \dots (4)$$

Where,  $KT$  is the temperature dependent constant,  $\eta$  be the viscosity.

#### **RESULT AND DISCUSSION :**

The Experimentally measured value of ultrasonic velocity, density and viscosity for the binary mixtures of 1- Heptanol and Acrylonitrile in different mole fractions at temperature 298K is given in table 1.

The values of acoustical parameters such as adiabatic compressibility, free length, Acoustic impedance, relaxation time at constant temperature 298K has been given in table 1.

The ultrasonic velocity increases with increase in a mole fraction of Acrylonitrile, which

indicates the presence of molecular association between solute and solvent. The variation of ultrasonic velocity in a mixture depends upon the increase or decrease of intermolecular free length, on the basis of a model for propagation proposed by Eyring and Kincaid [8]. The increase in velocity may be due the structural changes of molecules in the mixture take place due to the existence of electrostatic field between the interacting molecules. The density of mixture increases with concentration due to the presence of large number of molecules in the mixture. The viscosity increases in the system, suggesting thereby more association between solute and solvent molecules.

The adiabatic compressibility decreases with increasing concentration which shows that there is strong interaction between the molecules of liquid mixture. Also, the variation in intermolecular free length with mole fraction this decrease in free length is due to the decreased adiabatic compressibility which brings the molecules to a closer packing [9-10]. Acoustic impedance increases with increase in a concentration of acrylonitrile. Acoustic impedance shows opposite behavior as that of adiabatic compressibility and intermolecular free length.

Relaxation time ( $\tau$ ) increases with increasing mole fraction of the solute in this system. It represents that there is molecular interaction between the 1-Heptanol and acrylonitrile [11-13].

#### **CONCLUSION :**

The ultrasonic velocity, density, viscosity and other related parameters were calculated. The existence of molecular interaction in solute-solvent is favored in the system, confirmed from the U,  $\rho$ ,  $\eta$ ,  $\beta_a$ ,  $L_f$  and  $\tau$  data. The variation in ultrasonic velocity (U), density ( $\rho$ ) and viscosity ( $\eta$ ) and other related thermodynamic parameters such as  $\beta_a$ ,  $L_f$  and  $\tau$  at various concentrations and at 298K temperature in the 1- Heptanol in

Acrylonitrile shows the variation in linear Strong intermolecular interactions are confirmed in the systems investigated. This provides useful information about solute solvent interactions in the mixture as existing in the liquid system.

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**Table 1: Measured values of Ultrasonic velocity (U), density ( $\rho$ ) and viscosity ( $\eta$ ) and calculated values of Adiabatic compressibility ( $\beta_a$ ), free length ( $L_f$ ) and Relaxation time ( $\tau$ ) of 1- Heptanol in acrylonitrile at 298K and 2 MHz Frequency.**

Mole fraction of 1- Heptanol in Acrylonitrile	U (m/s)	$\rho$ (kg/m <sup>3</sup> )	$\eta \cdot 10^{-3}$ (CP)	$\beta_a \cdot 10^{-10}$ (Pa <sup>-1</sup> )	$L_f \cdot 10^{-10}$ (m)	$Z \cdot 10^6$	$\tau \cdot 10^{-12}$ (s)
0	1189	789.0	0.4018	8.9651	0.6163	0.9381	0.4802
0.1	1198.5	793.1	0.4290	8.7780	0.6098	0.9505	0.5021
0.2	1207	798.0	0.5301	8.6016	0.6036	0.9631	0.6079
0.3	1216.5	799.2	0.6850	8.4551	0.5985	0.9722	0.7722
0.4	1224	801.0	0.9272	8.3330	0.5941	0.9804	1.0301
0.5	1240.5	803.8	1.2360	8.0846	0.5852	0.9971	1.3323
0.6	1267.5	805.1	1.7380	7.7313	0.5723	1.0204	1.7916
0.7	1287.5	807.2	2.0770	7.4735	0.5627	1.0392	2.0696
0.8	1309	809.0	3.0486	7.2139	0.5528	1.0589	2.9323
0.9	1325	812.1	3.8540	7.0138	0.5451	1.0760	3.6042
1.0	1335.5	815.0	5.4722	6.8794	0.5398	1.0884	5.0194