



Research Article

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## Acoustic parameter investigation of ternary mixture of n-butanol, water and acetic acid by using ultrasonic technique

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### ABSTRACT

Ultrasonic velocity, Density and Viscosity for ternary mixture of n-Butanol, Water and Acetic acid ( $C_4H_9OH+H_2O+CH_3COOH$ ) (which is used as running solvent for TLC in peptide and peptidomimetic synthesis) have been measured at a constant temperature 289K at different concentrations by using Ultrasonic Technique. From experimentally obtained data other Acoustical parameters like Adiabatic Compressibility, Adiabatic Impedance, Intermolecular Free Length, Available Free Volume, Relaxation Time, Ultrasonic Attenuation, Wada's constant, Rao's constant, Vander waal's constant, Internal Pressure, Gibb's Free Energy and Enthalpy have been calculated. In this non-ideal mixture, non-linear variation of acoustical parameter with composition of the chemical system suggests the presence of weak molecular interaction.

**Key words:** Ternary mixture, Ultrasonic velocity, Intermolecular interactions, Gibb's Free Energy

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### INTRODUCTION

In recent years, ultrasonic technique has provided a fascinating approach to investigate the Acoustical parameters for a liquid system either binary or ternary; or pure liquid. A large number of studies have been made which are based on this particular technique but still there is a large scope of study. This kind of investigation gives information about molecular interactions, molecular structure and arrangement of molecules inside the liquid system used [1][2][4]. This information is interpreted by investigating the behavior of acoustical parameters in terms of concentrations or temperature. For ideal liquid mixture or a pure liquid the variation in parameters is supposed to be linear. But in case of non-ideal liquid mixture or unlike mixtures, it shows considerable departure from linearity. And this departure explains the existence of strong or dispersive interactions [3].

The present study deals with the measurement of ultrasonic velocity, density, viscosity and computation of other acoustical parameters for different concentrations at a constant temperature 289K and constant frequency range 2MHz by using Ultrasonic technique. In this experimental setup ternary mixture of n-Butanol, Water and Acetic Acid is used. This particular mixture is widely used as a running solvent in Thin Layer Chromatography (TLC) for Peptides, Amino acids and many other chemicals to monitor the progress of a reaction. The whole study is interpreted in terms of molecular interactions in the system of chemicals. By observing the trends of ultrasonic velocity, density and viscosity; the nature of chemical system cannot be defined so some other derived parameters such as adiabatic compressibility, acoustic impedance, intermolecular free length, ultrasonic attenuation, relaxation time, Wada's constant, Rao's constant, Vander Waal's constant, internal pressure, Gibb's free energy and enthalpy were calculated. The trends of these parameters can define the nature and behavior of a system more accurately.

### EXPERIMENTAL SECTION

The chemicals are obtained from Loba Chemicals of minimum assay of 99.9% and fresh distilled water is used throughout the investigation as a reference liquid and as one of the component of system also. The whole experiment is done at constant temperature of 289 K. For the measurement of ultrasonic velocity, ultrasonic interferometer (Mittal Enterprises-F-80 model) at a standard frequency range of 2 MHz with an accuracy of  $\pm 0.1$  m/s is used. The density and viscosity are measured with the help of Specific Gravity Bottle (25 ml, accuracy  $\pm 0.1$  kg/m<sup>3</sup>) and Ostwald's Viscometer (10 ml, accuracy 0.1%) respectively.

#### 3 Theory

The standard acoustical parameters are obtained experimentally. Other acoustical parameters are derived with the help of standard parameters and can be defined as,

##### Wada's constant

$$W = \frac{M}{\rho v \beta} \quad (1)$$

##### Rao's constant

$$R = \frac{MU^{1/3}}{\rho} \quad (2)$$

##### Vander Waals' constant

$$b = V \left[ 1 - \left( \frac{RT}{MU^2} \right) \left\{ \left( 1 + \frac{MU^2}{3RT} \right)^{\frac{1}{2}} - 1 \right\} \right] \quad (3)$$

##### Internal pressure

$$P = bRT \left[ \left( \frac{K\eta}{U} \right)^{1/2} \left( \frac{\rho^{2/3}}{M^{7/6}} \right) \right] \quad (4)$$

##### Gibb's free energy

$$\Delta G = K_B T \ln \left[ \frac{K_B T \tau}{h} \right] \quad (5)$$

##### Enthalpy

$$H = V_m P \quad (6)$$

Where  $K_T$  is temperature dependent Jacobson's constant,  $K$  is temperature independent constant,  $R$  is universal gas constant,  $K_B$  is Boltzmann constant,  $h$  is Planck's constant and  $U_\infty$  is Schaaf's limiting value.

### RESULTS AND DISCUSSION

The experimental values of ultrasonic velocity, density and viscosity for different concentrations of ternary mixture of n-Butanol, water and acetic acid at constant temperature 289 K and at constant frequency 2MHz are presented in Table-1. From the experimentally measured standard parameters Adiabatic Compressibility, Intermolecular Free Length, Acoustic Impedance, Relaxation Time and Ultrasonic Attenuation are calculated. The values are shown in Table-2. Table-3 gives values of Effective Molecular Weight, Free Volume, Wada's Constant and Rao's Constant. The values of Molar Volume, Available Volume, Vander Waal's Constant, Internal Pressure, Gibb's Free Energy and Enthalpy of the chemical system are given in Table-4.

**Table-1: Experimental values of ultrasonic velocity, density and viscosity**

Mole Fraction		Ultrasonic Velocity (U) (m/s)	Density ( $\rho$ ) (kg/m <sup>3</sup> )	Viscosity ( $\eta$ ) (kg/ms) (10 <sup>-3</sup> )
X <sub>1</sub>	X <sub>2</sub>			
0.50	0.33	1238	929.958	2.275
0.53	0.30	1363	926.586	2.025
0.57	0.26	1356	916.644	1.795
0.60	0.23	1348	900.391	1.831
0.63	0.20	1338	898.230	1.693
0.66	0.17	1340	891.746	1.879
0.70	0.13	1322	891.573	1.787
0.73	0.10	1306	876.185	2.043
0.77	0.06	1287	882.150	1.610
0.80	0.03	1278	862.461	1.590

**Table-2: Calculated values of adiabatic compressibility, intermolecular free length, acoustic impedance, relaxation time and ultrasonic attenuation**

Mole Fraction		Adiabatic Compressibility ( $\beta$ ) (N/m <sup>2</sup> ) (10 <sup>-10</sup> )	Intermole-cular Free Length (L <sub>f</sub> ) (Å°)	Acoustic Impedance (Z) (kg/m <sup>2</sup> s) (10 <sup>5</sup> )	Relaxation Time ( $\tau$ ) (s) (10 <sup>-12</sup> )	Ultrasonic Attenuation ( $\alpha/f^2$ ) (s <sup>2</sup> /m) (10 <sup>-14</sup> )
X <sub>1</sub>	X <sub>2</sub>					
0.50	0.33	7.018	0.5554	11.513	2.129	3.390
0.53	0.30	5.811	0.5054	12.629	1.569	2.269
0.57	0.26	5.935	0.5107	12.430	1.420	2.065
0.60	0.23	6.112	0.5183	12.137	1.492	2.083
0.63	0.20	6.219	0.5228	12.018	1.404	2.069
0.66	0.17	6.246	0.5240	11.950	1.565	2.303
0.70	0.13	6.418	0.5311	11.787	1.529	2.281
0.73	0.10	6.693	0.5424	11.443	1.823	2.752
0.77	0.06	6.845	0.5485	11.353	1.469	2.251
0.80	0.03	7.097	0.5585	11.022	1.505	2.332

**Table-3: Values of effective molecular weight, free volume, Wada's constant an Rao's constant**

Mole Fraction		Effective Molecular Weight (M) (gm/mol)	Free Volume (V <sub>f</sub> ) (m <sup>3</sup> /mol) (10 <sup>-7</sup> )	Wada's Constant (W) (m <sup>3</sup> /mol)(Pa) <sup>1/7</sup> (10 <sup>-3</sup> )	Rao's Constant (R) (m <sup>3</sup> /mol)(m/s) <sup>1/3</sup> (10 <sup>-4</sup> )
X <sub>1</sub>	X <sub>2</sub>				
0.50	0.33	53.14	0.1756	1.160	6.136
0.53	0.30	54.80	0.2531	1.234	6.560
0.57	0.26	57.06	0.3196	1.295	6.890
0.60	0.23	58.74	0.3212	1.351	7.207
0.63	0.20	60.42	0.3727	1.390	7.412
0.66	0.17	62.10	0.3328	1.438	7.677
0.70	0.13	64.34	0.3709	1.484	7.920
0.73	0.10	66.02	0.3096	1.541	8.236
0.77	0.06	68.26	0.4552	1.577	8.417
0.80	0.03	69.94	0.4760	1.644	8.800

**Table-4: Values of molar volume, available volume, Vander Waal's constant, internal pressure, Gibb's free energy and enthalpy**

Mole Fraction		Molar Volume (V <sub>m</sub> ) (m <sup>3</sup> /mol) (10 <sup>-5</sup> )	Available Volume (V <sub>a</sub> ) (m <sup>3</sup> /mol) (10 <sup>-5</sup> )	Vander Waal's Constant (b) (m <sup>3</sup> /mol) (10 <sup>-5</sup> )	Internal Pressure (P) (N/m <sup>2</sup> ) (10 <sup>7</sup> )	Gibb's Free Energy ( $\Delta G$ ) (KJ/mol) (10 <sup>-21</sup> )	Enthalpy (H) (J/mol)
X <sub>1</sub>	X <sub>2</sub>						
0.50	0.33	5.714	1.293	5.292	6.623	10.172	3784.254
0.53	0.30	5.916	0.876	5.513	5.909	8.955	3496.270
0.57	0.26	6.225	0.949	5.805	5.501	8.559	3424.509
0.60	0.23	6.524	1.027	6.087	5.480	8.755	3575.089
0.63	0.20	6.727	1.102	6.278	5.256	8.512	3575.424
0.66	0.17	6.964	1.131	6.505	5.481	8.945	3817.039
0.70	0.13	7.216	1.254	6.742	5.349	8.853	3860.245
0.73	0.10	7.535	1.385	7.040	5.664	9.554	4267.563
0.77	0.06	7.738	1.514	7.230	5.059	8.694	3915.024
0.80	0.03	8.109	1.632	7.580	4.950	8.788	4014.311

The value of ultrasonic velocity is measured at frequency 2MHz at different mole fractions. It decreases with increase in concentration of n-Butanol. It can be observed from figure 4.1. This is due to the increase in

Intermolecular Free length and the Adiabatic Compressibility [5] This behavior is different from the ideal mixture behavior and this can be attributed to the molecular association and structural changes occurring in the system [6].

Variation of viscosity and density is shown in the Figure 4.2 and 4.3. Density is a measure of solvent-solvent and ion-solvent interactions. Non-linear behavior is observed and shows decreases with increase in mole fraction. Decrease in density emphasizes the lesser magnitude of solute-solvent interactions. It indicates weak molecular interaction between the chemical components [7].

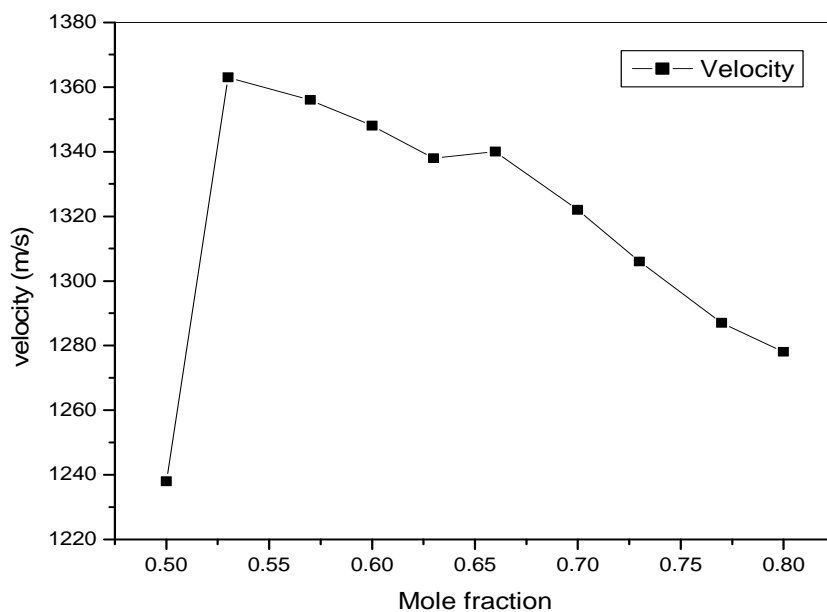


Figure 4.1: Ultrasonic velocity versus mole fraction at temperature 289 K

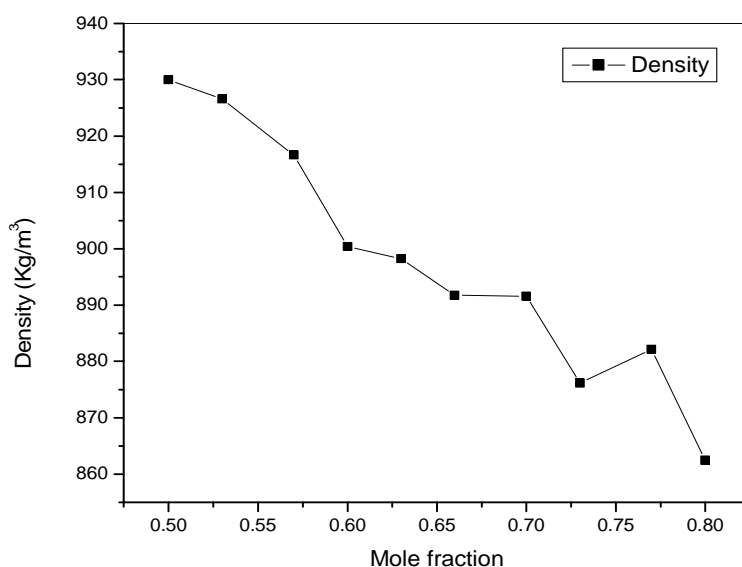


Figure 4.2: Density versus mole fraction at temperature 289 K

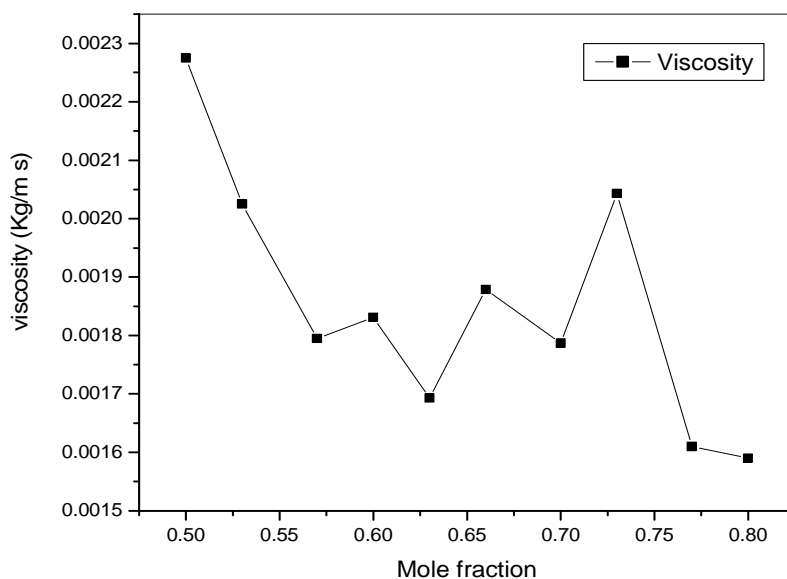


Figure 4.3: Viscosity versus mole fraction at temperature at 289 K

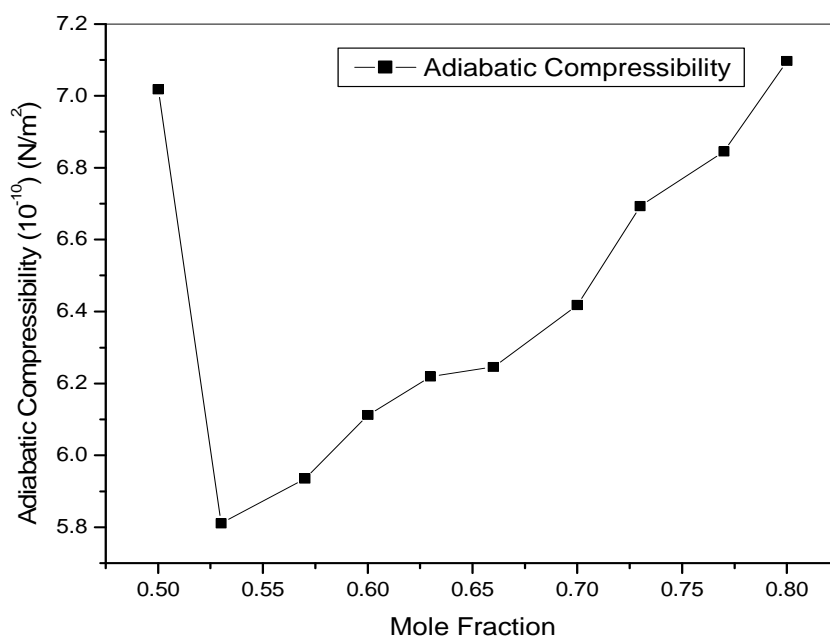


Figure 4.4: Adiabatic Compressibility versus Mole Fraction at temperature 289 K

It is clear from the Table-2 that Acoustic Compressibility and Intermolecular Free Length increases with increase in mole fraction. Both parameters are inversely proportional to the square of Ultrasonic Velocity. The trends of plots in figure 4.4 and 4.5 are also just opposite to that of Ultrasonic Velocity. The increase in free length is due to the loose packing of the molecules in the system, which interprets the presence of weak molecular interactions.

Figure 4.6 illustrate the non-linear behavior of Acoustic Impedance with mole fraction. It exhibits opposite trend as compared to Adiabatic Compressibility. This is another evidence of the presence of weak molecular

interactions. Relaxation Time decreases with increase in mole fraction. From Figure 5.7, trend of this parameter versus mole fraction can be noted. The best results are obtained between 0.63 to 0.70 ranges of mole fraction. This behavior is due to molecular rearrangement in the mixture and the reason for this is co-operative processes. Figure 4.8 emphasize that Ultrasonic Attenuation shows similar behavior as Relaxation Time shows. It is a non-linear pattern. Ultrasonic attenuation is the decay rate of the wave as it propagates through material.

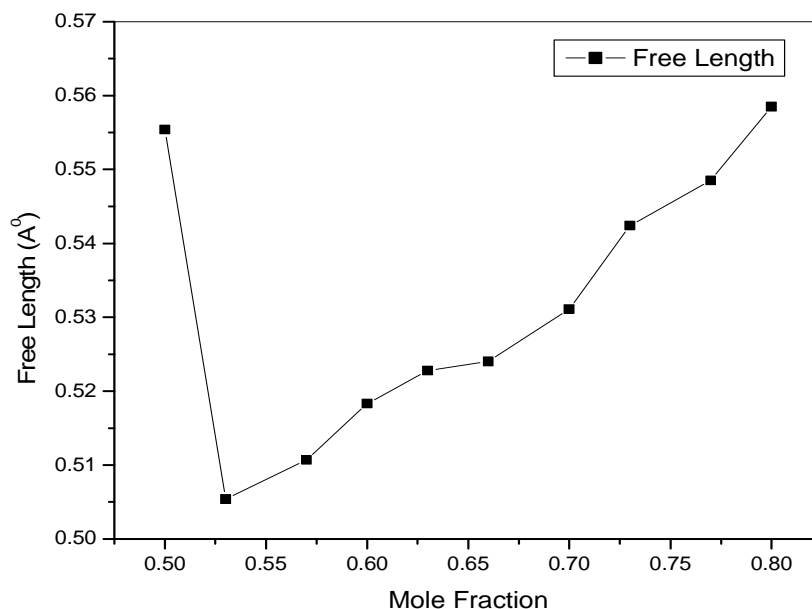


Figure 4.5: Inter-molecular Free Length versus Mole Fraction at temperature 289 K

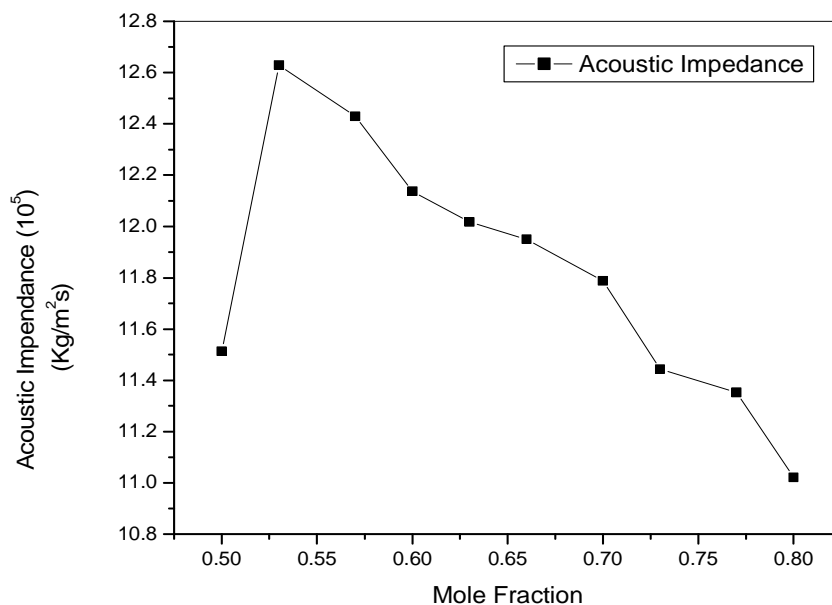
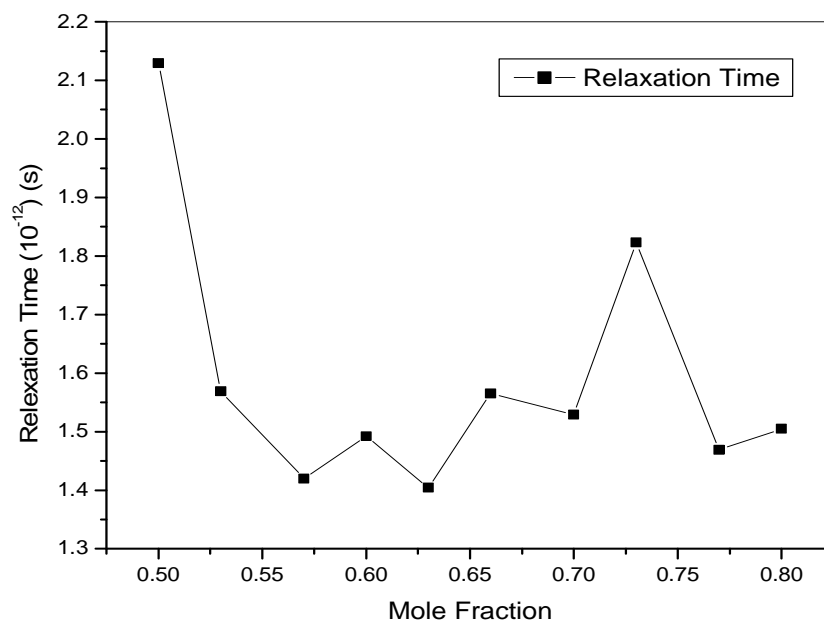
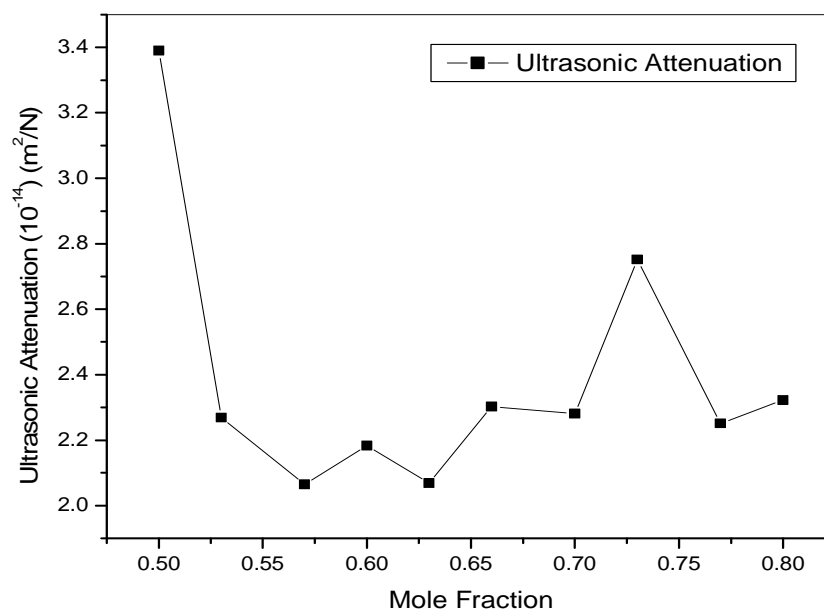


Figure 4.6: Acoustic Impedance versus Mole Fraction at temperature 289 K

**Figure 4.7: Relaxation Time versus Mole Fraction at temperature 289 K****Figure 4.8: Ultrasonic Attenuation versus Mole Fraction at temperature 289 K**

Free Volume increases with increase in mole fraction as shown in figure 4.9. Free Volume represents the average volume in which the center of the molecules can move inside the cell due to the repulsion of surrounding molecules [8]. The best trend can be observed between 0.63 to 0.70 ranges of mole fraction. Figure 4.10 and Figure 4.11 shows that Wada's Constant and Rao's Constant increase with increase in mole fraction. The trends are almost linear and this signifies the absence of complex formation in the experimental chemical system.

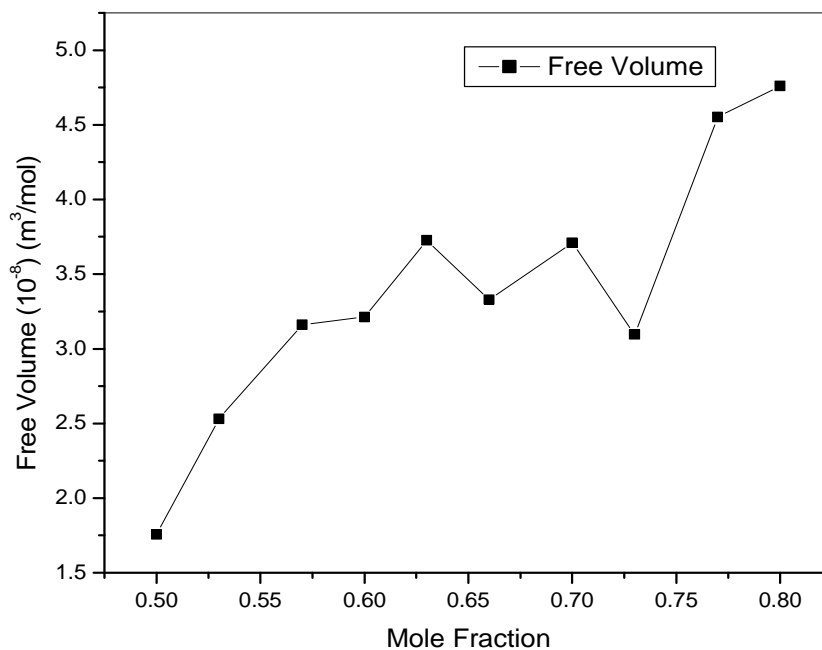


Figure 4.9: Free Volume versus Mole Fraction at temperature 289 K

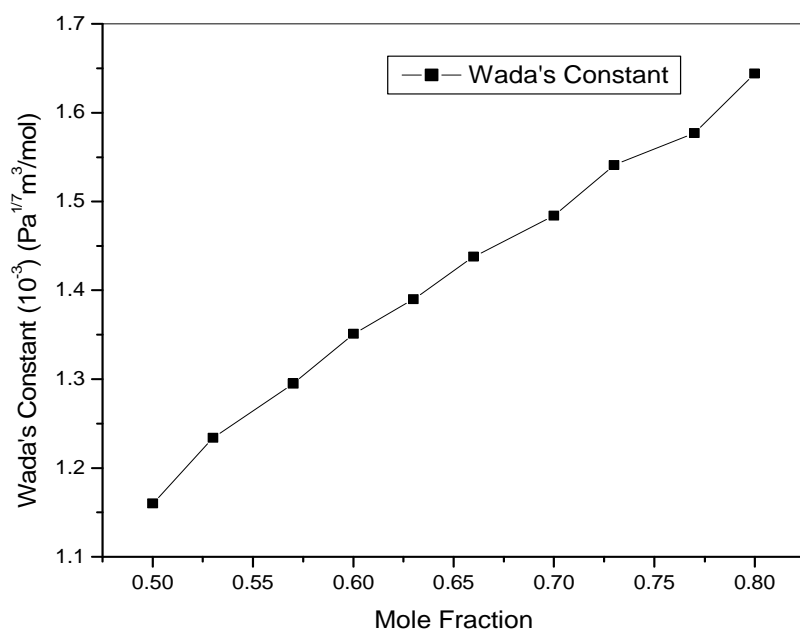


Figure 4.10: Wada's Constant versus Mole Fraction at temperature 289 K



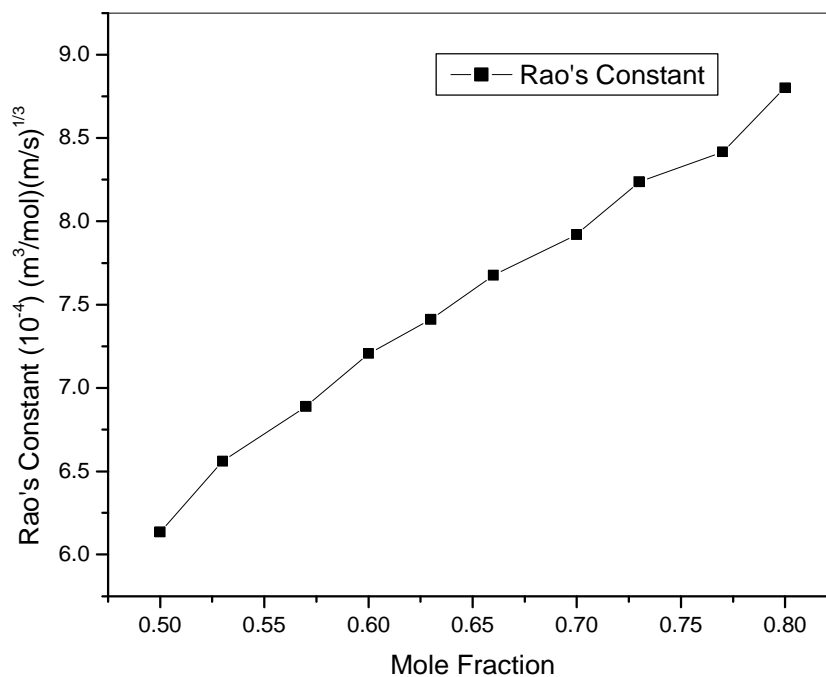


Figure 4.11: Rao's Constant versus Mole Fraction at temperature 289 K

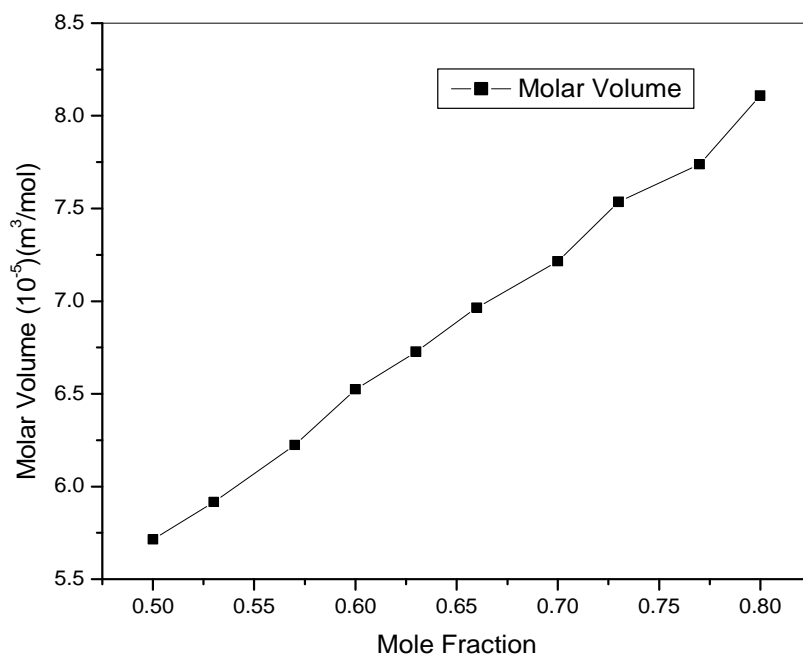


Figure 4.12: Molar Volume versus Mole Fraction at temperature 289 K

Figure 4.12 and Figure 4.13 shows almost linear variation of Molar Volume and Available Volume with mole fraction. As mole fraction increases, molar Volume and Available Volume also increase. Available Volume is a

direct measure of the compactness and strength of bonding between the molecules of the system [9]. Figure 4.14 emphasizes the variation of Vander Waal's Constant with mole fraction. Vander Waal's Constant is also called the Co-volume and varies in Vander Waal's Equation in the similar way as Available Volume does. Figure 4.15 unveils the relation between Internal Pressure and Mole Fraction. It shows that internal pressure decreases with increase in mole fraction. Exact trends can be noted between the mole fraction ranges from 0.63 to 0.70. This signifies that the solution becomes more compressible. The reduction in internal pressure shows dissociating tendency of the molecules in the solution.

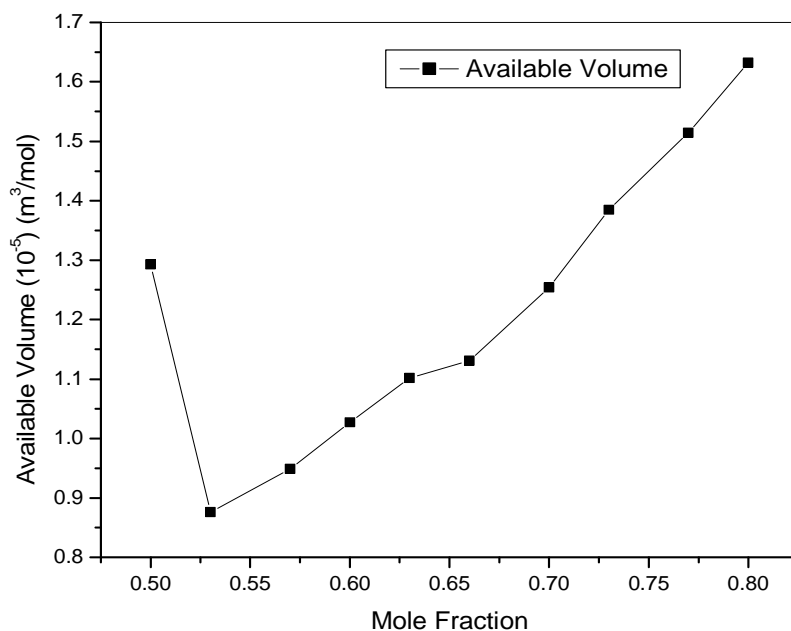


Figure 4.13: Available Volume versus Mole Fraction at temperature 289 K

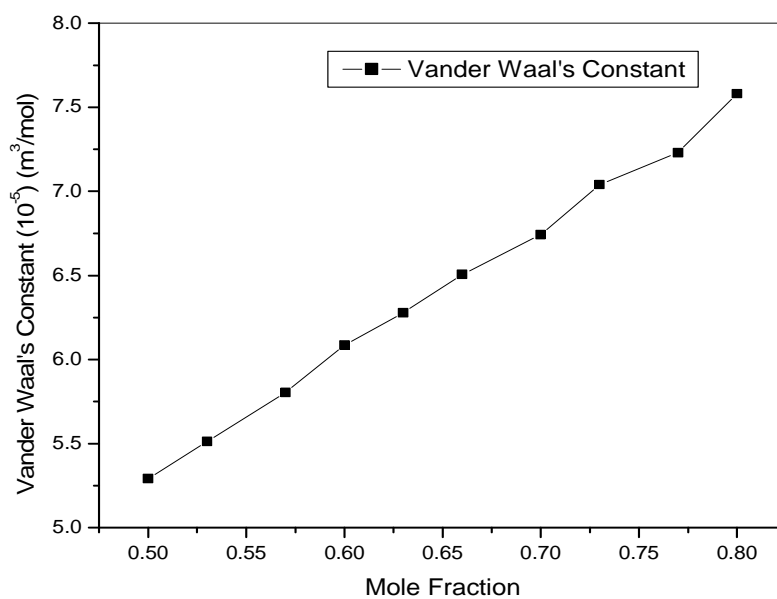


Figure 4.14: Vander Waal's Constant versus Mole Fraction at temperature 289 K

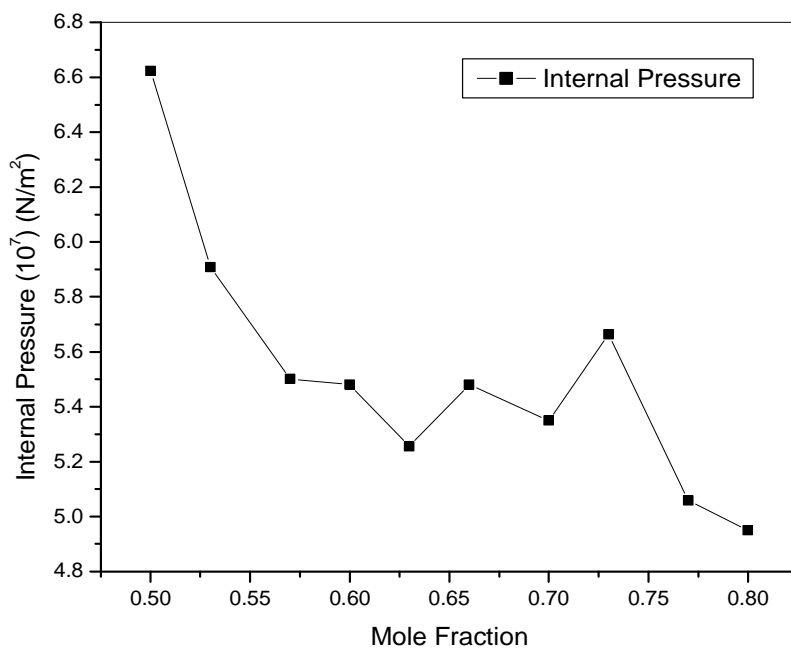


Figure 4.15: Internal Pressure versus Mole Fraction at temperature 289 K

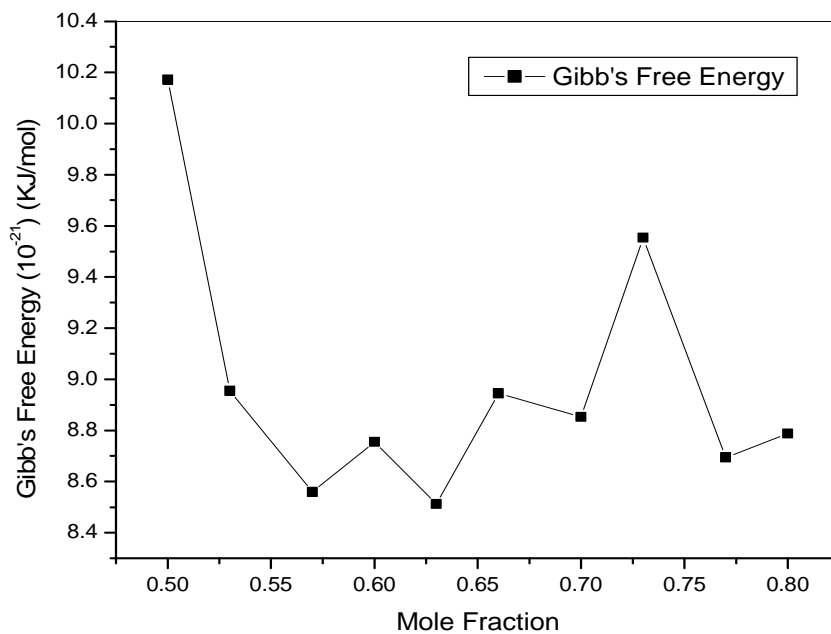


Figure 4.16: Gibb's Free Energy versus Mole Fraction at temperature 289 K

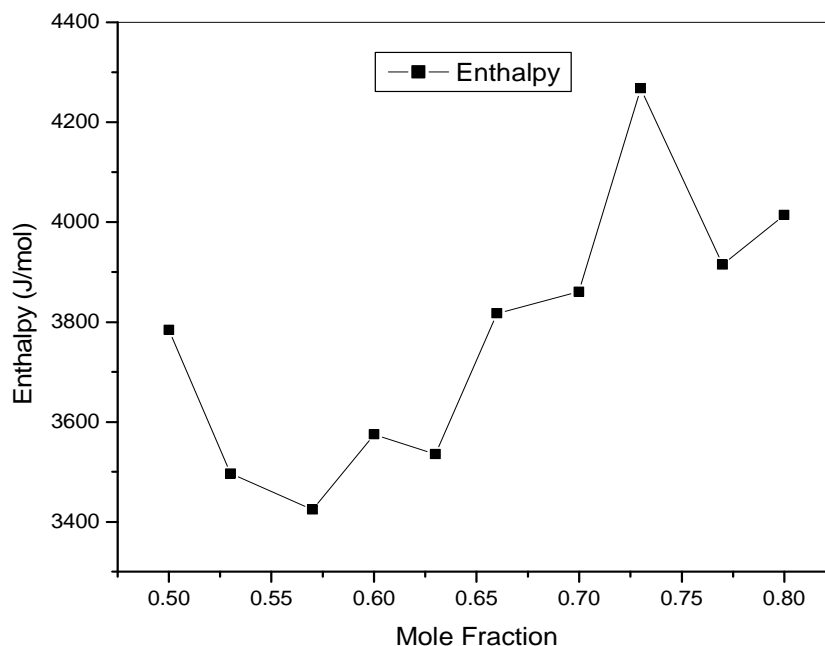


Figure 4.17: Enthalpy versus Mole Fraction at temperature 289 K

Figure 4.16 gives non-linear relation of Gibb's Free Energy with Mole fraction. It decreases as mole fraction increases. This observation confirms the formation of intermolecular hydrogen bonding in ternary chemical mixture. Also, it gives information about the completion of the reaction. Figure 4.17 shows the variation of Enthalpy with an increase in Mole Fraction.

### CONCLUSION

In present study, the ternary chemical mixture of n-Butanol, Water and Acetic Acid forms a non-ideal liquid mixture which shows considerable departure from linearity from their physical properties with respect to mole fraction. In this particular mixture presence of weak intermolecular interaction between unlike molecules is signified. Also there is solvent-solvent interaction present in the system. Complex formation in the system is completely declined. By observing the plots it can be concluded that this ternary mixture shows best results in the mole fraction range from 0.63 to 0.70. Thus between this concentration ternary mixture of n-Butanol, Acetic Acid and Water can be used as a running solvent in TLC.

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