ULTRASONIC STUDY OF MOLECULAR INTERACTION IN BINARY LIQUID MIXTURE CONTAINING TRIETHYLAMINE IN ACETONITRILE AT 305.15K

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Abstract

Ultrasonic velocity and absorption measurements in binary liquid mixture as a function of the concentration and concentration are useful in gaining insight into the structure and bonding of associated molecular complexes and other molecular processes occurs in these liquid mixtures. The results observed in these ultrasonic measurements have been correlated with molecular interactions in liquid mixtures with some degree of success. The absorption and velocity of sound in binary mixtures of triethylamine with Acetonitrile have been measured at a central frequency of 5MHz, using the interferometer. Ultrasonic absorption peaks at intermediate concentrations have been found in a binary mixture. In this work, measurements of the velocity, absorption coefficient, density, adiabatic compressibility, excess compressibility, and shear viscosity as functions of the concentration are reported. The adiabatic compressibility and excess compressibility were calculated from the velocity and the density measurements. The ultrasonic velocity (u), density (ρ) and viscosity (η) have been measured for the binary mixtures of triethylamine with Acetonitrile at 305.15K. From the experimental data, Adiabatic Compressibility (β), Free Length (L_f), Free Volume (V_f)), Internal Pressure (π_i), Acoustic Impedance (Z), and Cohesive Energy(H) have been calculated. In addition to that the excess values of certain above parameters are also computed. These excess parameters have been used to discuss the presence of significant molecular interactions in binary mixture. By taking measurements at several concentrations of each liquid mixture, we obtained information about the molecular association between the two different molecules in the liquid mixture.

KEY WORDS: Magnetic fluid, ultrasonic velocity, density, viscosity, thermo-acoustic parameters, and intermolecular interactions.

INTRODUCTION:

Now-a-days ultrasonic is an area of intense scientific and technological research. In view of its extensive scientific and engineering applications it attracts attention of researchers, non- destructive testing professionals, industrialists, technologists, medical practitioners, instrumentation engineers, software engineers and medical scientists. The study of ultrasonic waves in pure and liquid mixtures is useful to examine the nature of intermolecular interactions occurred in these liquids. The various acoustic parameters such as ultrasonic velocity, density, viscosity, adiabatic compressibility, free length, acoustic impedance, relaxation time, free volume and internal pressure are useful in understanding molecular structure and molecular interactions in the medium[1-3].

Recent development in science and technology for non – destructive technique are spectacular and holds significant possibilities for better new applications in molecular structure, molecular interactions, medicines and underwater acoustics. Development of sensors, electronic instrumentation and computer software added sophistication to the experimental and theoretical agreement of different ultrasonic parameters [4-7]. Thermodynamics studies of binary liquid mixtures have attracted much attention of scientists. These physico-chemical analyses are used to handle the mixtures of hydrocarbons, alcohols, aldehydes, ketones etc. The measurement of ultrasonic speed enables us to the accurate measurement of some useful acoustic and thermodynamic parameters and their excess values [8-13]. These excess values of ultrasonic velocity, adiabatic compressibility, molar volume and viscosity in binary liquid mixture are useful in understanding the solute-solvent interactions. The study of molecular association in binary liquid mixture having alcohol as one of component is of particular interest since alcohols are strongly self associated liquids having three dimensional network of hydrogen bonding and can be associate with any other group having some degree of polar attraction [14-16]. The variation in ultrasonic velocity gives information about the bonding between molecules and formation of complexes at various concentration and temperature through molecular interactions [17-19]. In order to have clear understanding of intermolecular interaction between component molecules of an attempt has been made to study the ultrasonic behaviors of triethylamine in Acetonitrile at different temperature. Thermo-acoustic parameters are the essential sources of information for better understanding of non-ideal behavior of complex binary liquid system [20-22].

EXPERIMENTAL:

The chemicals triethylamine and Acetonitrile used were of analytical grade and obtain from Merck chemicals private Ltd. (Purity 99.5%). The densities of pure components and binary mixtures were measured by hydrostatic sinker method with an accuracy 1 part in10^{+5}. Special attention was given to avoid the vaporization of solution. Comparing their density with literature values checked the purity of chemicals. The mixtures of various concentrations in mole fraction were prepared. The ultrasonic velocities in pure liquids and their mixtures have been measured by ultrasonic interferometer supplied by Mittal Enterprises, New Delhi at a central frequency of 5 MHz with accuracy ± 0.01 m/s. The viscosity of pure and mixture is measured by an Ostwald/s Viscometer with accuracy ± 0.001 $Nm^{-}s$. The temperature of pure liquids and their mixtures is maintained constant temperature water bath with an accuracy of ± 0.01K.

THEORYTICAL ASPECT:

The adiabatic compressibility (β) has been calculated from sound velocity ‘u’ and the density (ρ) of the medium using the relation

$$\beta = \frac{1}{u^2 \rho} \qquad (1)$$

Intermolecular free length (L_f) has been determined by the equation.

$$L_f = K_T \sqrt{\beta} \qquad (2)$$

Where K_T is a Jacobsen's constant.

The free volume L_f in terms of ultrasonic, velocity (u) and the viscosity (η) of a liquid is

$$V_f = \left(\quad \right)^{3/2} \qquad (3)$$

Where M_{eff} is the effective molecular weight

$$M_{eff} = \sum \quad x_i \qquad (4)$$

In which mi & xi are the molecular weights and mole fraction of individual constituents respectively and K is a temperature dependent constant equal to 4.28×10^9 for all liquids in MKS system.

Specific acoustic impedance (Z) is determined from equations,

$$Z = u \cdot \rho \qquad (5)$$

Where 'u' and 'ρ' are the ultrasonic velocity and density of the mixture respectively.

RESULTS AND DISCUSSION:

Ultrasonic velocity (u), density (ρ), viscosity(η) and other related excess thermodynamic parameters are evaluated for binary mixture triethylamine(TEA) in Acetonitrile over whole concentration at 301.15 K, 305.15 K .

In the binary liquid systems under investigation, the variation of ultrasonic velocity (u), density (ρ), viscosity (η), Adiabatic Compressibility (β), Acoustic Impedance (Z), and molar volume (V_m) are shown in Fig-I, Fig-II, Fig-III, Fig-IV, Fig-V and Fig-VI. The variation of these acoustic parameters indicate the existence of molecular interaction between solvent and solute optimum at specific concentration and it may leads to formation weak hydrogen bonded complex in binary liquid mixture.

Table-1: For binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K.

Mole Fraction (x)	u (ms^{-1})	$\eta\times10^{-3}$ (Nsm^{-2})	$\beta_a\times10^{-7}$ (m^2n^{-1})	Z ($Kgm^{-2}\ s^{-1}$)	$V_m\times10^3$ (m^3)
0.0	1260.0	0.4018	8.1654	0.9719	53.2149
0.1	1246.6	0.4073	8.4337	0.9511	61.6828
0.2	1232.0	0.4090	8.7332	0.9294	70.3579
0.3	1218.0	0.4155	9.0140	0.9108	79.0211
0.4	1197.0	0.4155	9.4162	0.8872	87.8386
0.5	1188.0	0.4154	9.6113	0.8755	96.4993
0.6	1170.0	0.4174	9.9756	0.8567	105.3340
0.7	1152.2	0.4176	10.3172	0.8412	113.8858
0.8	1143.3	0.4096	10.5332	0.8303	122.7619
0.9	1128.0	0.4077	10.8778	0.8149	131.7315
1.0	1110.0	0.4096	11.3039	0.7969	140.9331

Table-2: For binary liquid mixture containing Triethylamine in Acetonitrile at 305.15K.

Mole Fraction (x)	u (ms^{-1})	$\eta\times10^{-3}$ (Nsm^{-2})	$\beta_a\times10^{-7}$ (m^2n^{-1})	Z ($Kgm^{-2}\ s^{-1}$)	$V_m\times10^3$ (m^3)
0.0	1190.0	0.3670	9.2417	0.9092	53.7233
0.1	1177.0	0.3690	9.5621	0.8885	62.3446
0.2	1160.2	0.3699	9.9678	0.8646	71.2169
0.3	1147.0	0.3745	10.2772	0.8483	79.8972
0.4	1130.0	0.3748	10.6652	0.8297	88.6640
0.5	1117.0	0.3740	10.9776	0.8155	97.4113
0.6	1100.0	0.3784	11.4087	0.7968	106.4798
0.7	1083.1	0.3740	11.8361	0.7800	115.4513
0.8	1070.0	0.3715	12.1513	0.7691	124.0428
0.9	1057.0	0.3663	12.5182	0.7557	133.1133
1.0	1034.0	0.3699	13.1143	0.7374	141.8817

Table-3: For binary liquid mixture containing Triethylamine in Acetonitrile at 309.15K.

Mole Fraction (x)	u (ms^{-1})	$\eta \times 10^{-3}$ (Nsm^{-2})	$\beta_a \times 10^{-7}$ (m^2n^{-1})	Z ($Kgm^{-2}\ s^{-1}$)	$V_m \times 10^3$ (m^3)
0.0	1118.0	0.3481	10.52	0.8502	53.9776
0.1	1107.0	0.3500	10.8934	0.8292	62.8273
0.2	1090.0	0.3517	11.3679	0.8070	71.6882
0.3	1077.0	0.3566	11.7136	0.7926	80.2880
0.4	1056.6	0.3566	12.2787	0.7707	89.2474
0.5	1047.0	0.3529	12.5964	0.7582	98.2049
0.6	1030.0	0.3587	13.0662	0.7430	106.9227
0.7	1017.0	0.3557	13.4996	0.7283	116.0961
0.8	1000.2	0.3513	13.9784	0.7152	124.6847
0.9	989.0	0.3466	14.3732	0.7034	133.8057
1.0	970.5	0.3502	14.9685	0.6883	142.6618

Table-4: For binary liquid mixture containing Triethylamine in Acetonitrile at 313.15K.

Mole Fraction (x)	u (ms^{-1})	$\eta \times 10^{-3}$ (Nsm^{-2})	$\beta_a \times 10^{-7}$ (m^2n^{-1})	Z ($Kgm^{-2}\ s^{-1}$)	$V_m \times 10^3$ (m^3)
0.0	1049.0	0.3421	12.0079	0.7938	54.2415
0.1	1037.0	0.3381	12.4720	0.7731	63.1223
0.2	1022.0	0.3354	13.0029	0.7524	72.0874
0.3	1009.0	0.3382	13.4738	0.7355	81.0589
0.4	989.2	0.3421	14.0726	0.7183	89.6529
0.5	981.0	0.3364	14.4040	0.7076	98.5860
0.6	966.6	0.3421	14.9671	0.6912	107.8646
0.7	949.2	0.3381	15.5731	0.6764	116.6662
0.8	938.0	0.3359	15.9854	0.6669	125.4037
0.9	929.2	0.3340	16.3771	0.6571	134.5814
1.0	912.5	0.3362	17.0278	0.6435	143.4709

This conclusion is further supported by thermodynamic studies [11, 16] on a similar system by IR and NMR [18-24]. Beyond this optimum concentration, addition of solute (triethylamine) in a solvent (Acetonitrile) tries to break this weak complex structure and tends towards the values of pure components.

Figure -I: Variation of Ultrasonic Velocity with mole fraction for binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K, 305.15K, 309.15K, 313.15K.

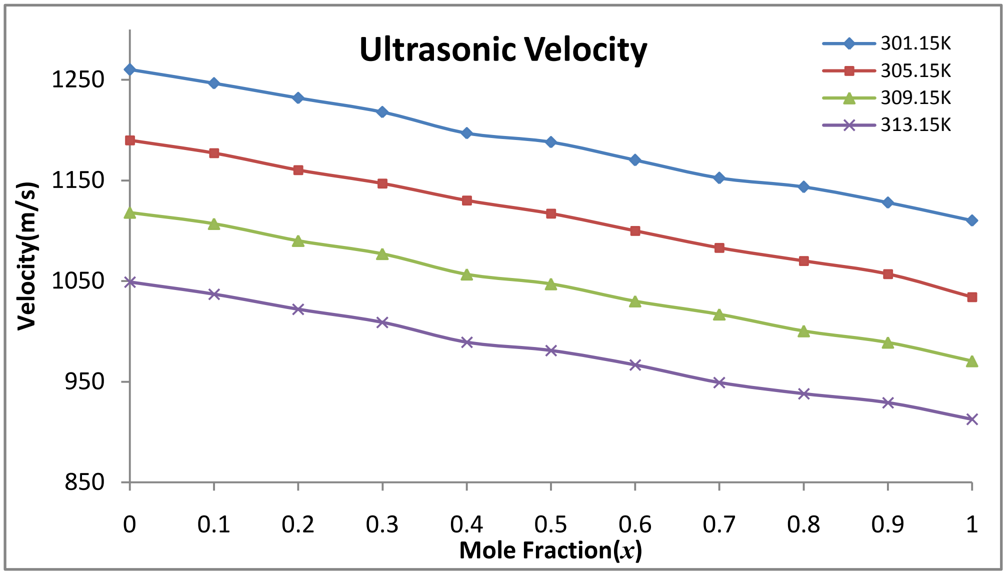


Figure -II: Variation of Density mole fraction for binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K, 305.15K, 309.15K, 313.15K.

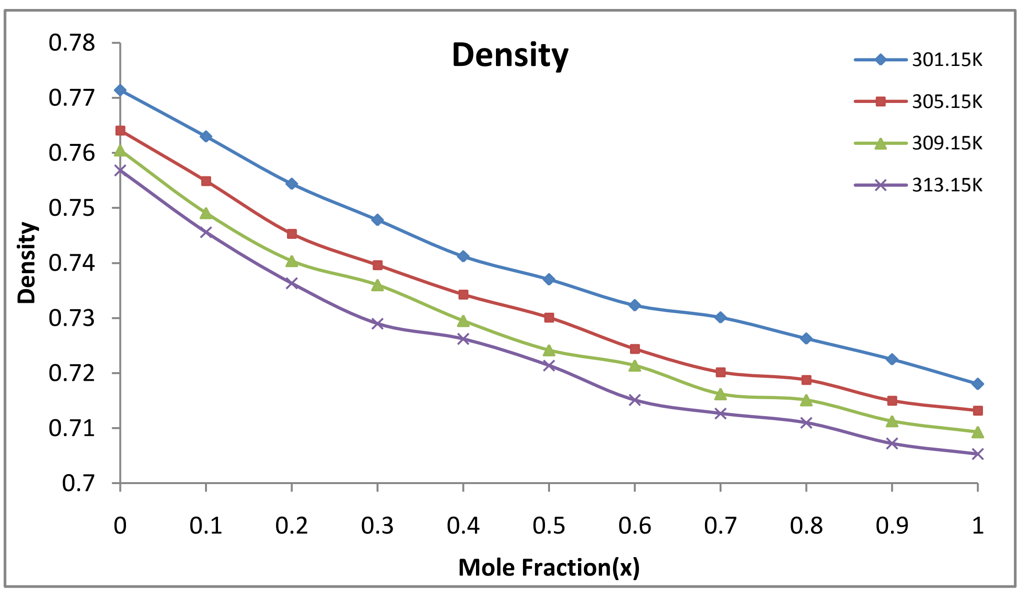


Figure-III: Variation of Viscosity with mole fraction for binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K, 305.15K, 309.15K, 313.15K.

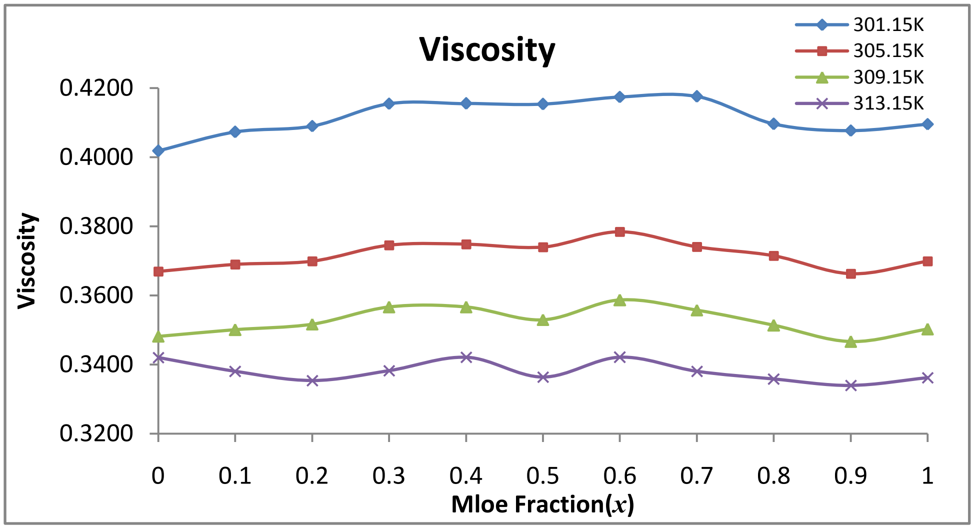


Figure-IV: Variation of Adiabatic Compressibility with mole fraction for binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K, 305.15K, 309.15K, 313.15K.

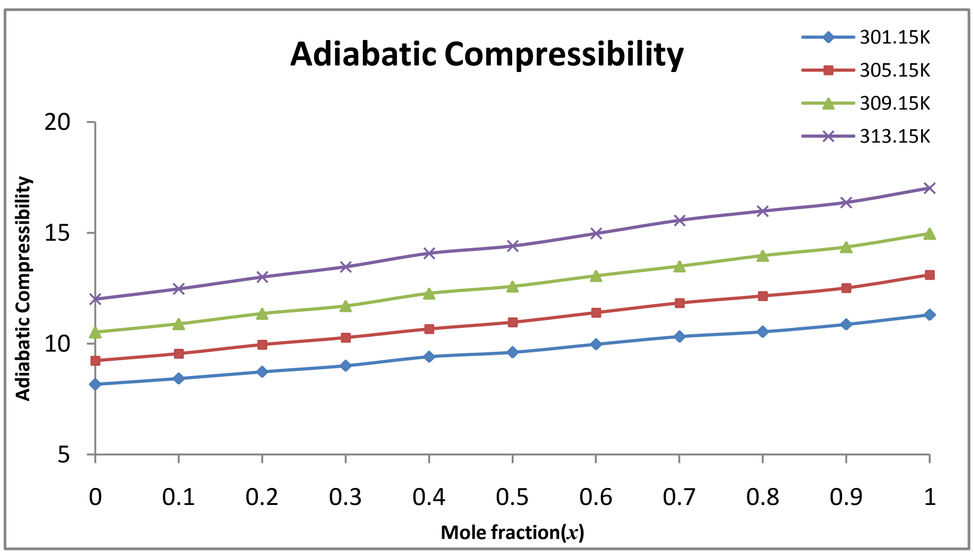


Figure-V: Variation of Acoustic Impedance with mole fraction for binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K, 305.15K, 309.15K, 313.15K.

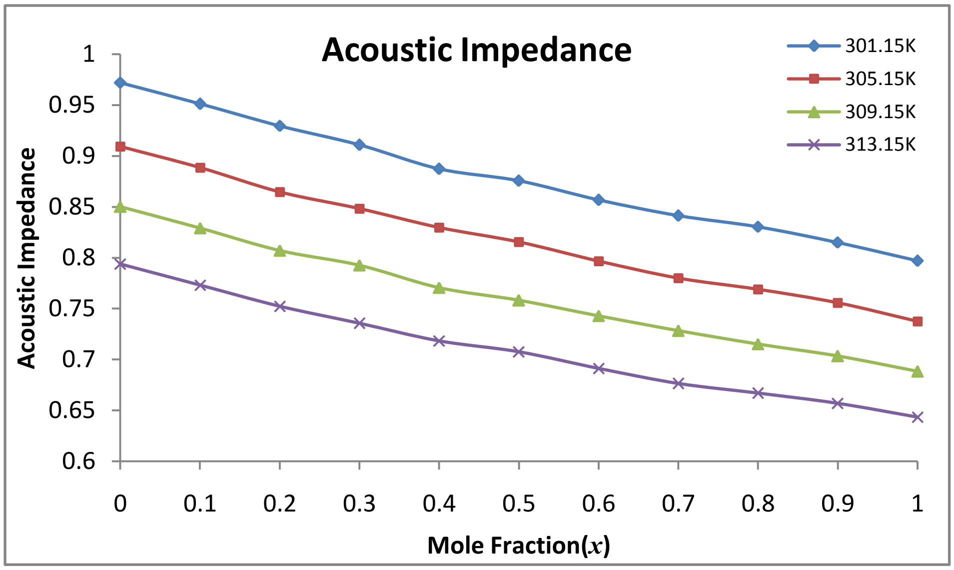
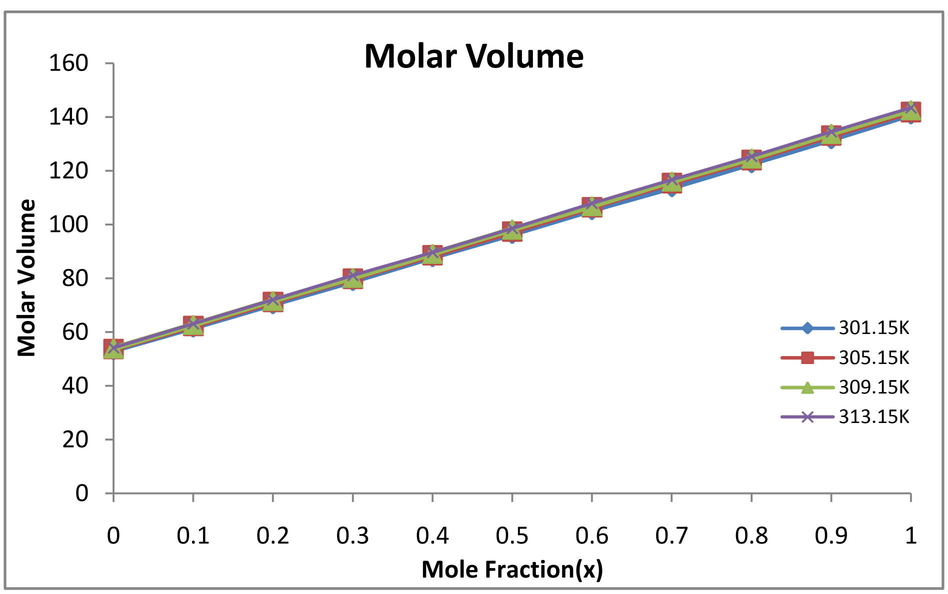


Figure-VI: Variation of Molar Volume with mole fraction for binary liquid mixture containing Triethylamine in Acetonitrile at 301.15K, 305.15K, 309.15K, 313.15K.



CONCLUSION:

The acoustic data of Ultrasonic velocity (*u*), viscosity (*η*), Adiabatic Compressibility (*β*), Acoustic Impedance (*Z*) and molar volume (V_m) of Triethylamine in Acetonitrile over the whole concentration range may suggest the existence of a strong intermolecular interaction.

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