Molecular Interactions Study of Acetone and Aniline 303k

Prashant B Dabrase[1], B M Suryavanshi[2], R A Patil, P.R.Kakde[3]

[1, 3]Bhalerao Science College, Saoner (M.S.) India

Dept of Physics, Government Institute of Science, Nagpur (M.S.) India

[2]S.S.S.K.R.Innani Mahavidyalaya, Karanja (lad), (M. S.) India

Abstract: *The ultrasonic study is proving to be a simple and easy technique to determine the basic properties of the liquid and liquid mixtures. The behaviour of the molecules in the liquids with its neighbour is very important while preparing liquids or solutions for the various applications. The measurements of Ultrasonic velocity (υ) with density (ρ) and viscosity (η) are carried out to find out the different ultrasonic parameters with varying composition of the binary system at temperature 303K. The results have been discussed and graphically presented. All the plots of ultrasonic velocity (υ), viscosity (η), compressibility (β), intermolecular free length (L_f) and acoustic impedance (Z), free volume (V_f), internal pressure (π_i) at temperature 303K indicates an intermolecular interaction between the components of the mixture. The importance of excess values never be neglected and they provides details of the strength of the any existing interactions. Therefore the excess values of the above parameters are also evaluated and the results are discussed.*

Keywords: velocity, Compressibility, free length, internal pressure, molecular interaction, excess parameters

1. Introduction

There are so many studies available for investigating the nature of intermolecular interaction and the different forces but Ultrasonic studies have always played an important role in the study of liquids and liquid mixtures. These ultrasonic investigations of liquid mixtures are important in understanding the physical nature and strength of molecular interaction. The ultrasonic velocity of liquid is basically related to the bonding forces between the atoms and molecules. It helps to understand the nature of molecular interactions in pure and binary mixtures of the liquids [1-5]. Many researchers have studied the binary mixtures of the various compounds but it is observed that a little attempt has been made to study the ultrasonic and thermodynamic properties of aromatic polar compounds like Aniline. The Aniline and Acetone which are having many applications in pharma-industries from drugs preparation to its solubility and also in many applications such as bio-medical, chemical and industrial are used here. These liquids & their mixtures are of interest to organic chemists to know about the type of bond and number of each molecule in the formation of complexes [6-7]. It is important to discuss the different parameters in terms of their excess values rather than actual in order to understand the nature of molecular interactions between the components of the liquid mixtures.

In the present study the ultrasonic velocity, density and viscosity measurements have been carried out for various concentrations of aniline at temperature 303K. The variations of different ultrasonic parameters and their excess values are studied to understand molecular interactions.

2. Experimental

The chemicals Aniline and Acetone were obtained commercially of AR grade with purity of 99.5% and used without further purification. The binary mixture for varying mole fraction of aniline was prepared at room temperature and preserved in a specially designed air tight container. The mixture so prepared is utilised within 24 hours of its preparation. Ultrasonic velocities (υ) for different concentrations of pure liquids and binary mixtures were measured on Ultrasonic Interferometer at 1 MHz (Mittal enterprises- model M-81). The density measurements were carried out by using volumetric study. The viscosities have been measured using the constant flow viscometer. The experimentally measured density (ρ) in kgm^{-3}, ultrasonic velocity (υ) in ms^{-1} and viscosity (η) in Nsm^{-2} are used to evaluate various parameters by using the standard relations such as,

Adiabatic Compressibility (β_α), $\beta_\alpha = 1 / \upsilon\rho$ --------------1,
Intermolecular free length (L_f) $L_f = K\beta_\alpha^{1/2}$ -------------2,
Acoustical Impedance (Z) $Z = \rho\ \upsilon$ -------------3,

Where, K –is temperature dependant constant and T – absolute temperature [8],

Free volume (V_f), $V_f = \left[\dfrac{M_{eff}\upsilon}{\eta\kappa}\right]^{3/2}$ -------------- 4,

where, M_{eff} is the effective molecular weight ($M_{eff} = \Sigma m_i X_i$), k is temperature independent constant which is equal to 4.28 X 10^9 for all liquids.

The internal pressure (π_i),

$\pi_i = bRT\left[\dfrac{\eta\kappa}{\upsilon}\right]^{1/2}\left[\dfrac{\rho^{2/3}}{M_{eff}^{7/6}}\right]$ -------------- 5,

where, k is a constant, T is the absolute temperature, b is a constant equal to 2 for the liquid and the excess values of these parameters are determined by using the relation

$A^E = A_{exp} - A_{id}$ -------------- 6,

A^E - excess value of any acoustic parameters, $A_{id} = \sum_{i=1}^{n} A_i X_i$,

International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064, Impact Factor (2013): 4.438
www.ijsr.net

A_i is any acoustical parameter and X_i – the mole fraction of liquid component.

3. Result and Discussion

The graphical representation of the data obtained from the measurements and evaluation of various parameters is given in figure1. The values of ultrasonic velocity (υ) and density (ρ) increases with the concentration of Aniline in the binary mixture of Aniline and Acetone. But the adiabatic compressibility (β_α) decreases sharply at 303K temperature. Free length (L_f) is also showing similar relation to that of compressibility for the increasing concentration of Aniline in the mixture. The values of viscosity (η), acoustical impedance and internal pressure (π_i) are seen to be increasing with the concentration of aniline in the mixture. The concentration of aniline in the mixture increases this naturally imbalances the space available for the molecules of acetone. This is because of the size and charge distribution of the aniline. The acetone tries to occupy the interstitial spaces and therefore the cohesive force between the components of the mixture increases which results in decreasing the intermolecular free length and therefore the internal pressure of the mixture as a whole increases, figure (1-8). The decrease in free length is also responsible for the available space for the molecules to vibrate and therefore the free volume in this case appears to be decreasing. It is clear that intermolecular free length depends upon intermolecular attractive and repulsive force [9].This suggests the close packing of the molecules, which may be concluded as the increasing magnitude of the interaction[10].
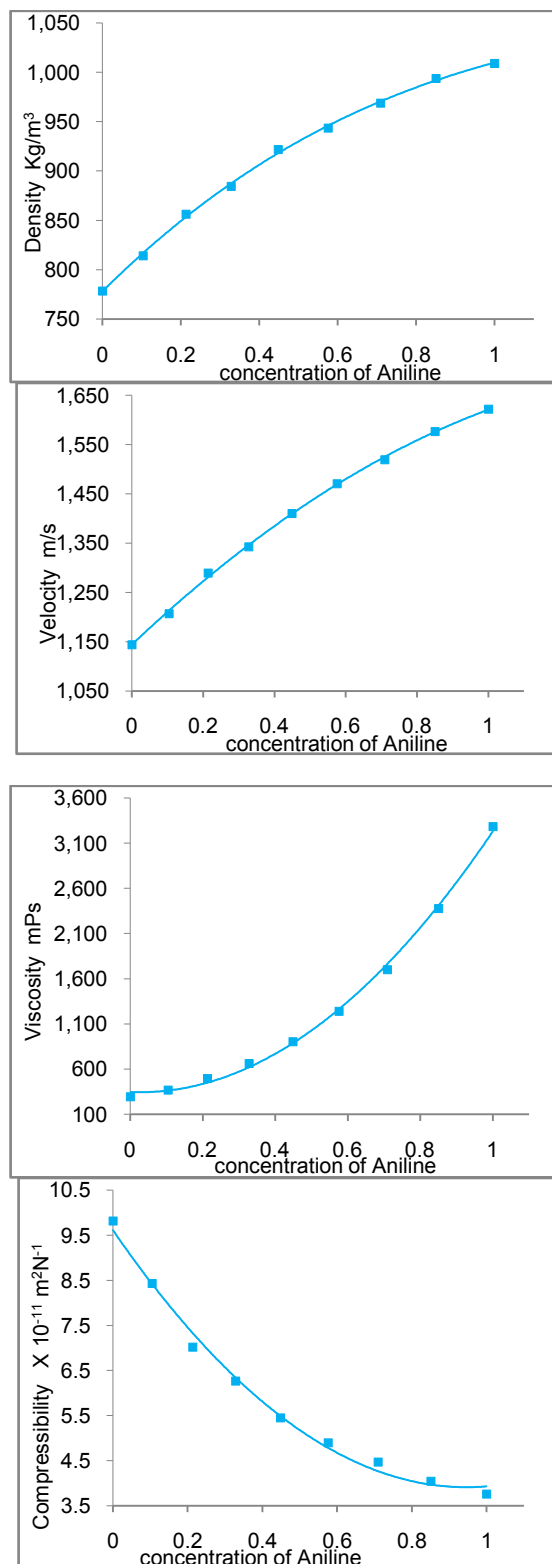
The plots of these parameters with concentrations conforms the non linear variation (figure 01-08). The values of adiabatic compressibility (β_α) and free length (L_f) decreases with increase in the concentration of Aniline. The decrease in the values of free length with increasing concentration can be concluded being a significant interaction between the two liquids [11].
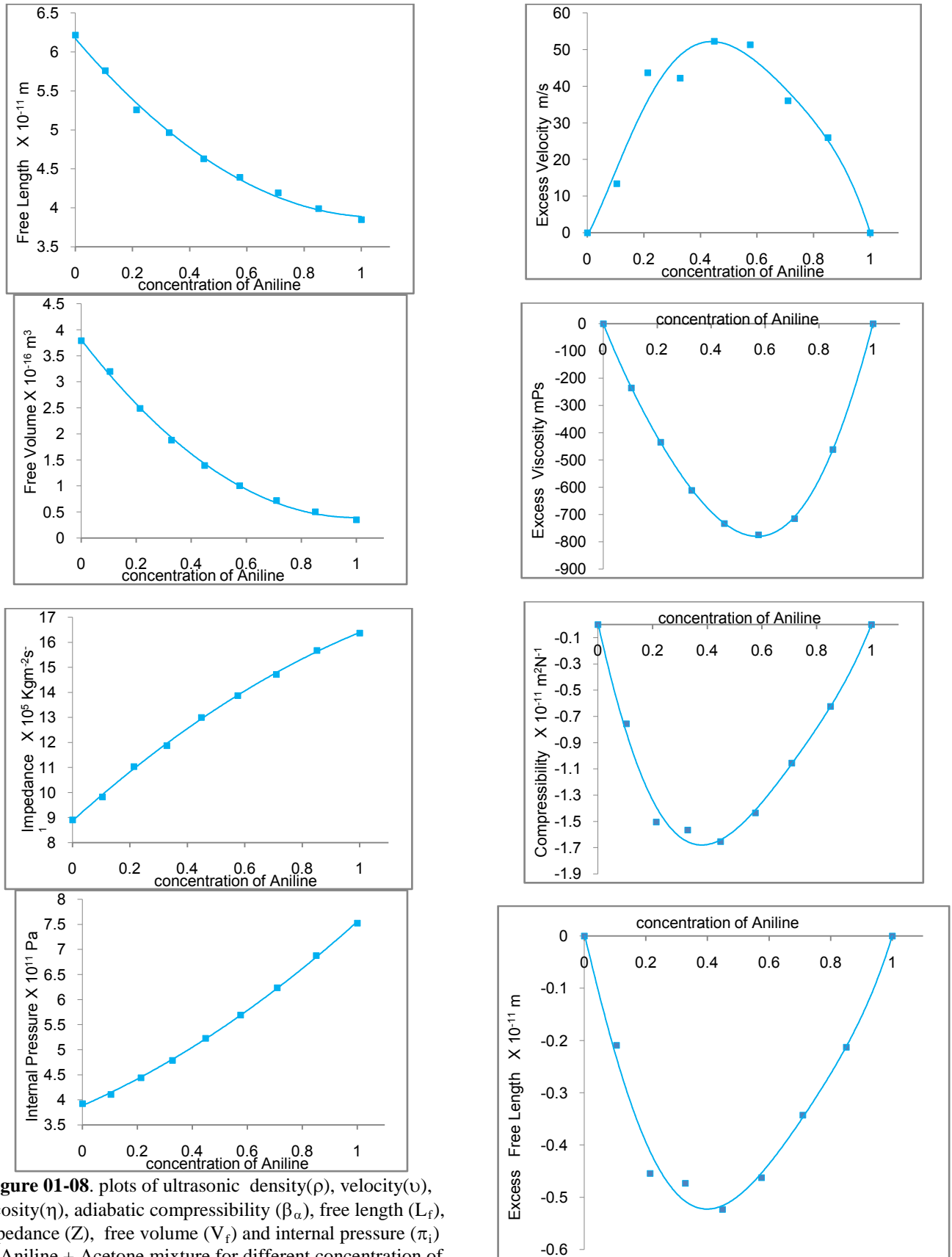
The viscosity is the parameter which depends on the frictional forces between molecules any variation in the viscosity is due to a change in effective molecular area and resulting cohesive or adhesive forces or relative random velocity between the components of the mixture [12].

The extent of deviation & sign of the excess functions determines the strength of interaction between unlike molecules [13, 14]. The nature of excess velocity is seen to be positive which can be concluded as the presence of interaction. The excess compressibility and free length shows the negative nature and the same trend can be observed in the excess values of viscosity it means the strong attractive or repulsive forces are acting between the different components of the mixture. It is known that the dipoles when interact with the other dipole the intermolecular free length increases or decreases accordingly and the compactness of the structure decreases the free length. Therefore the negative value of excess free length, excess volume and internal pressure are negative, this can be confirmed from the figure 8-15. The excess value of impedance is observed to be positive. It means resistance to the mechanical vibrations
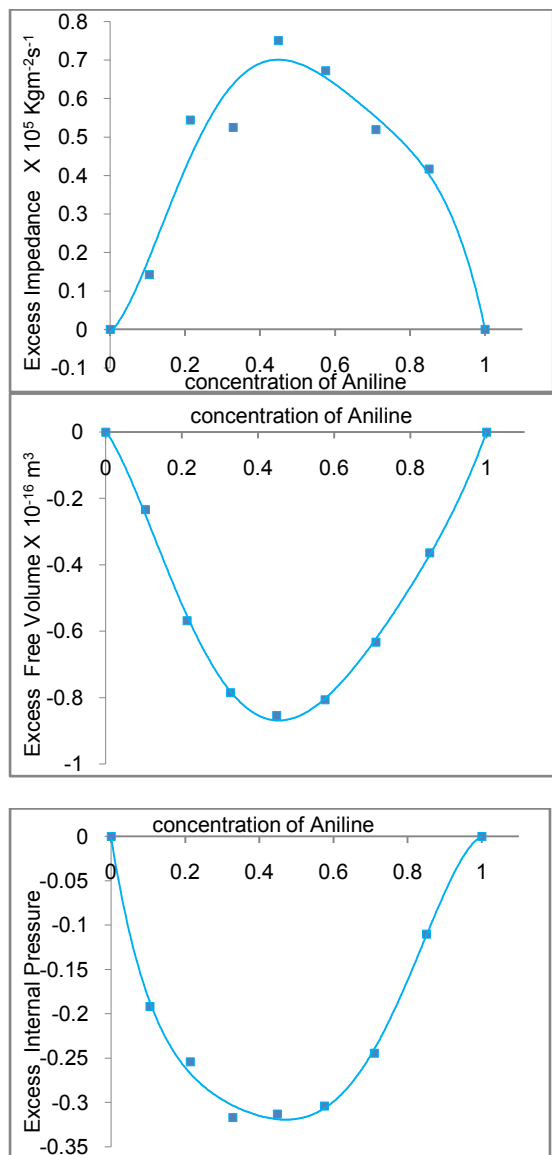
increases with the increase in concentration of Aniline in the mixture.

3.1 Figures

International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064, Impact Factor (2013): 4.438
www.ijsr.net

Figure 01-08. plots of ultrasonic density(ρ), velocity(υ), viscosity(η), adiabatic compressibility (β_α), free length (L_f), impedance (Z), free volume (V_f) and internal pressure (π_i) for Aniline + Acetone mixture for different concentration of Aniline at 303K temperatures.

International Symposium on Ultrasonics-2015, 22-24 January 2015
Department of Physics, Rashtrasant Tukdoji Maharaj Nagpur University, Nagpur, Maharashtra, India
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International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064, Impact Factor (2013): 4.438
www.ijsr.net

Figure 09-15. plots of excess values of ultrasonic velocity (υ^E), viscosity(η^E), adiabatic compressibility ($\beta_\alpha{}^E$), free length ($L_f{}^E$), impedance (Z^E) free volume ($V_f{}^E$) and internal pressure ($\pi_i{}^E$) with their excess values for Aniline + Acetone mixture for different concentration of Aniline at 30K temperatures.

4. Conclusion

The evaluated parameters of the binary liquid mixture of Aniline and Acetone at 303 K in the present study lead to conclude the existence of interaction between the different molecules of the compounds in the mixture. The positive values of excess ultrasonic velocity (υ^E), and excess impedance and the negative excess values of viscosity (η^E), compressibility ($\beta_\alpha{}^E$), free length ($L_f{}^E$), free volume ($V_f{}^E$) and internal pressure ($\pi_i{}^E$) for the different concentration of the aniline in the mixture conforms the presence of strong dipole-dipole, dispersive, structure making interaction between the components of the mixture. The excess values of thermodynamic parameters are sensitive to the molecular interaction present in the liquid mixture. The interaction is predominant at 0.4 to 0.5 of mole fraction of aniline in the binary mixture.

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