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## RESEARCH ARTICLE

# ULTRASONIC INVESTIGATION OF ANILINE + 1-HEXANOL+ BENZENE AT 303 K

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## ABSTRACT

The velocity, density and viscosity of ternary system are determined over the entire range of composition at 303K from the calculated data’s, thermal parameter as adiabatic compressibility (β), free length ($L_f$), free volume ($V_f$) and internal pressure ($\pi_i$) have been evaluated using standard relations. The results are predicted molecular interaction between the components of the ternary combination. Observed excess values provide in all the mixtures indicates that molecular package, the specific interaction and nature of liquid mixtures. The presence of strong dipole-induced dipole, dipole-dipole type interaction was confirmed in the ternary system.

## INTRODUCTION

The association and forecast of properties of multicomponent mixtures through models and procedure (Acree, 1986). Which use information from the properties of their integral ternary mixtures is an area of research in evaluation within the general study of the liquid states. Velocity of sound waves in a channel is elementally related to the unbreakable forces between the atoms or the molecules (Venkatesu *et al*, 1977).

In recent years much Endeavour has been made with the competition and elucidation of the ultrasonic properties of liquids, and liquid mixtures (Oswal at al, 2004). The ultrasonic studies are of great significance in helping to understand the nature and extent of the patterns of molecular aggregation that exist in liquid mixtures, resulting from the intermolecular interaction (Lloukhani *et al*, 2003). The study of molecular interaction is said in the organic ternary combinations [aniline ($C_6H_5NH_2$) + 1-Hexanol ($C_6H_{13}OH$) +benzene ($C_6H_6$)] is distinct interest as it demands alcohol as one of the component. Aniline is stable and highly polar, and its seems to be best among the various extractive solvents due to its highly boiling point(457.4k) and structural features (Reddick *et al*,1986).

The capacity of aniline in fragment the various binary azeotropes has been studied by many researchers using different techniques (Arul *et al*,2005).Benzene is a non-polar, being aromatic and also aniline aromatic with amino group act as electron donors (Kincaid *et al*,1938). Though the amino is comparatively a strong electron-donor, the H atoms in the $NH_2$ group can also play the role of electron-acceptor centers, hence 1-Hexanol with its hydrophobic and hydrophilic groups can interact with other two components, if the components behave as electron-donors, in these case the hydrophobic is attractive type interaction and the hydrophilic shows repulsive type whereas repulsive interaction exist in between the two electron–donors, as a net consequence of ternary system experiences a larger compressibility. In case of if aniline behave as electron-acceptor then it seems that donor-acceptor complexation of the two solutes exists in the alcohol medium. Wherein all are attractive type interaction that leads to a comparatively lower compressibility (Thiyagarajan *et al*, 2008; Mieczink *et al*, 2004)

Hence, the present work distribute with the assessment of ultrasonic velocity, density and viscosity and computation of related parameter at 303K in the ternary system of Aniline+1-Hexanol+Benzene.

### Experimental Details

The mixtures of various concentrations in mole fraction were prepared by taking AR grade chemicals, which were decontaminate by standard methods (Suryanarayana, 1979). In this system, the mole fraction of second component 1-Hexanol ($X_2$=0.3) was kept fixed while the mole fractions of the persisting two were varied from (0.0 to 1.0) so as to have the mixtures of different composition. There is nothing consequential on fixing the second component ($X_2$=0.3).The ultrasonic velocity (U) in liquid mixtures have been deliberated using an ultrasonic interferometer (Mittal type, Model F-80) working at 2 MHz fixed frequency with an accuracy of ± 0.1 $ms^{-1}$.The density (ρ) and viscosity (η) are deliberated using a pycknometer and an Ostwald’s viscometer respectively with an accuracy of 3 parts in $10^5$ for density and $0.001Nsm^{-2}$ for viscosity. Using the deliberated data, the acoustical restrictions such as adiabatic compressibility (β), free length ($L_f$), free volume ($V_f$) and internal pressure ($\pi_i$) and their excess restrictions have been enumerated using the following standard expressions (Arunbahl *et al*, 2005).

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$$B = (U^2\rho)^{-1} \tag{1}$$

$$L_f = K_T\beta^{1/2} \tag{2}$$

$$V_f = \left[\frac{M_{eff}U}{¦\,k}\right]^{\frac{3}{2}} \tag{3}$$

$$®_i = bRT\left[\frac{k¦}{U}\right]^{\frac{1}{2}}\left[\frac{\circ^{\frac{2}{3}}}{M^{\frac{7}{6}}{}_{eff}}\right] \tag{4}$$

$$A^E = A_{exp}-A_{id} \tag{5}$$

$$A_{id} = \Sigma x_i A_i \tag{6}$$

where, $K_T$ is the temperature dependent constant having a value $201.1209\times10^{-8}$ in MKS system, k is a constant equal to $4.28\times10^9$ in MKS system, unconventional of temperature for all liquids, b is the cubical packing fraction taken as 2 for all the liquids, R is the universal gas constant, T is the innovative temperature, $M_{eff} = \Sigma x_i m_i$ where, x is the mole fraction and m is the molecular weight of $i^{th}$ component and $A^E$ stands for excess property of any given parameter, $A_{exp}$ is the innovative value and $A_{id}$ is the ideal value (Sundharam *et al*, 2005).

**Formulae Used**

From the assessment data, adiabatic compressibility (β) and its excess values ($\beta^E$) were deliberated using the following standard expression (Palaniappan, 2001).

$$\beta = 1/\rho U^2$$
$$\beta^E = \beta_{exp} - \beta^{id}$$

The ideal adiabatic compressibility β (= $-(1/V^{id}m)/\ \partial V^{id}m/\partial \rho)s^{id}$ ), is deliberated from the usual thermodynamic relation (Douheret *et al*, 2005) having the ideal isothermal compressibility $K_T^{id}$, ideal isobaric expansibility $\alpha_p^{id}$ and the ideal molar heat capacitance σ and the experimental temperature T as

$$\beta^{id} = K_T^{id} - T(\alpha_p^{id})^2/\ \sigma^{id} \tag{1.2}$$

The deliberation of ideal amalgamate laws of thermodynamic Gibbsian properties (Reis *et al*, 2001) mandate that the isothermal compressibility, thermal expansibility and the heat capacitance should be delivered in terms of ideal volume fraction $\ddot{}_i$ and hence,

$$K_T^{id} = \sum_i \ddot{}_i K_{T,I} \tag{1.3}$$

$$\alpha_p^{id} = \sum_i \ddot{}_i \alpha_{p,I} \tag{1.4}$$

$$\sigma^{id} = \sum_i \ddot{}_i \sigma_i \tag{1.5}$$

As the molar volume $V_m$ and the molar isobaric heat capacity $C_{p,m}$ are mole fraction condiment, the heat capacitance or the heat capacity per unit volume for the components can be done as (Lide *et al*, 1994; Riddick *et al*, 1986).

$$\sigma = C_{p,m}/V_m$$

and the ideal volume fraction as

$$\ddot{}_i = (X_iV_i)/(\sum_i X_iV_i) \tag{1.7}$$

The respective prevailing principles of isothermal compressibility, isobaric expansibility and heat quantity for the components are taken from literature (Pandy *et al*, 2007; Palaniappan, 2008).

## RESULTS AND DISCUSSION

Measured values of density (ρ), viscosity (η) and velocity (U) at 303 K for the ternary system of Aniline+1-Hexanol+Benzene are given in Table I. All the measured restitutions increase with increasing mole fraction of aniline. Such linear distinction indicates the presence of intermolecular interactions between the components (Thiyagarajan *et al*, 2007).

Among the three components, aniline and 1-Hexanol are awaited to involve in strapping interaction due to their polar nature (Ali A *et al*, 2002). Even though benzene is unsaturated, it conducts like a saturated compound generally. Moreover, the presence of benzene molecules as electron donor will gives inflated stability to the carbocation of 1-Hexanol and hence they cannot provide any strong interaction. As Aniline is having comparatively higher dielectric constant (6.8012) then benzene (2.2620) and both are electron donors, the interaction linking the molecules of aniline with benzene is established to be stronger (Ernest L Eliel, 1985). The increasing trend of viscosity (η) revealed that the addition of aniline increases the constructive molecular area. The increase in area due to the inclusion of a cyclic molecule (Aniline) by substitute linear molecule (1-Hexanol) is fully abnormal (Eyring *et al*, 1938). This may be due to the polar nature of the added component and is reflected in the observed trend of the deliberated restitution.

(1)

(1.1)

**Table I** The merits of density (ρ), viscosity (η) and velocity (U) of the system: Aniline + 1-Hexanol+Benzene at 303 K

| **Molefraction** | | **ρ** | **η** | **U** |
|---|---|---|---|---|
| $X_1$ | $X_3$ | ($kgm^{-3}$) | ($\times10^3 Nsm^{-2}$) | ($ms^{-1}$) |
| 0.0000 | 0.7694 | 951.5 | 1.4074 | 1091.5 |
| 0.0764 | 0.6929 | 957.5 | 1.4338 | 1166.0 |
| 0.1536 | 0.6158 | 964.1 | 1.4613 | 1281.0 |
| 0.2307 | 0.5385 | 970.4 | 1.5063 | 1328.3 |
| 0.3079 | 0.4615 | 976.4 | 1.7040 | 1476.5 |
| 0.3849 | 0.3842 | 983.0 | 1.8131 | 1689.2 |
| 0.4616 | 0.3075 | 989.3 | 1.9150 | 1905.0 |
| 0.5388 | 0.2305 | 995.6 | 2.0545 | 2193.2 |
| 0.6025 | 0.1591 | 1001.9 | 2.2382 | 2203.0 |
| 0.6927 | 0.0768 | 1008.2 | 2.3137 | 2282.1 |
| 0.7050 | 0.0000 | 1014.5 | 2.4207 | 2310.2 |

The perusal of Table II disclose that adiabatic compressibility (β), intermolecular free length ($L_f$) and internal pressure ($\pi_i$) are continuously decreases with increasing mole fraction of aniline whereas free volume ($V_f$) is in increasing trend and a depletion in adiabatic compressibility is a symptom that component molecules are held close to each other. Thus, addition of aniline makes all the components to be very closer. This idea is supported by the decreasing trend of intermolecular free length ($L_f$).

Free volume ($V_f$) and internal pressure ($\pi_i$) are acting opposite to each other. Free volume ($V_f$) shows a increasing trend of 0.4 mole fraction, whereas 0.5 mole fraction is a decreasing trend of aniline. Since the π and σ electrons of benzene are readily available for an electrophile, it guides to a suggestion that weak dispersive types as well as dipole-induced dipole type interaction are ascendant between the benzene and other polar molecules.

The addition of aniline with a mixture guides to a opaque structure due to the presence of dipolar type interaction. This subscribes to increase in free volume values. However, as these can simply form multiplex structures, interior pressure shows on decreasing trend (Mahendran *et al*, 2011).

**Table II** The merits of adiabatic compressibility (β), free length ($L_f$), free volume ($V_f$) and internal pressure ($\pi_i$) of the system: Aniline + 1-Hexanol + Benzene at 303 K.

| **Molefraction** | | **β** | **$L_f$** | **$V_f$** | **$\pi_i$** |
|---|---|---|---|---|---|
| $X_1$ | $X_3$ | ($x10^{10}pa^{-1}$) | ($x10^{11}m$) | ($\times10^7m^3mol^1$) | ($\times10^{-8}$ Pa) |
| 0.0000 | 0.7694 | 8.8215 | 5.9262 | 0.5881 | 6.3629 |
| 0.0764 | 0.6929 | 7.6818 | 5.5301 | 0.6465 | 6.3120 |
| 0.1536 | 0.6158 | 6.3209 | 5.0164 | 0.7384 | 6.0150 |
| 0.2307 | 0.5385 | 5.8405 | 4.8220 | 0.7603 | 5.9254 |
| 0.3079 | 0.4615 | 4.6970 | 4.3247 | 0.7853 | 5.9114 |
| 0.3849 | 0.3842 | 3.5652 | 3.7674 | 0.8574 | 5.6463 |
| 0.4616 | 0.3075 | 2.7853 | 3.3299 | 0.9659 | 5.4004 |
| 0.5388 | 0.2305 | 2.0881 | 2.8832 | 1.0943 | 5.1588 |
| 0.6025 | 0.1591 | 2.0565 | 2.8613 | 1.0974 | 5.0719 |
| 0.6927 | 0.0768 | 1.9044 | 2.7535 | 1.1088 | 5.0562 |
| 0.7050 | 0.0000 | 1.8469 | 2.7116 | 1.2872 | 5.0058 |

**Table III** The Excess Value of adiabatic compressibility ($\beta^E$), free length ($L_f^E$), free volume ($V_f^E$) and internal pressure ($\pi_i^E$) of the system: Aniline +1-hexanol + benzene at 303 K

| **Molefraction** | | **$L_f^E$** | **$V_f^E$** | **$\pi_i^E$** |
|---|---|---|---|---|
| $X_1$ | $X_3$ | ($x10^{11}m$) | ($\times10^7m^3mol^{-1}$) | ($\times10^{-8}$ Pa) |
| 0.0000 | 0.7694 | 4.7412 | 0.5026 | -1.2977 |
| 0.0764 | 0.6929 | 0.5679 | 0.5015 | -1.8381 |
| 0.1536 | 0.6158 | 0.2336 | 0.5332 | -1.8935 |
| 0.2307 | 0.5385 | 0.0392 | 0.4950 | -1.7336 |
| 0.3079 | 0.4615 | -0.3675 | 0.4599 | -1.4970 |
| 0.3849 | 0.3842 | -0.8350 | 0.4720 | -1.5139 |
| 0.4616 | 0.3075 | -1.1835 | 0.9213 | -1.5065 |
| 0.5388 | 0.2305 | -1.5397 | 0.5889 | -0.7610 |
| 0.6025 | 0.1591 | -1.4887 | 0.5430 | -0.5765 |
| 0.6927 | 0.0768 | -1.4895 | 0.4831 | -0.3688 |
| 0.7050 | 0.0000 | -1.1953 | 0.6590 | 0.2414 |

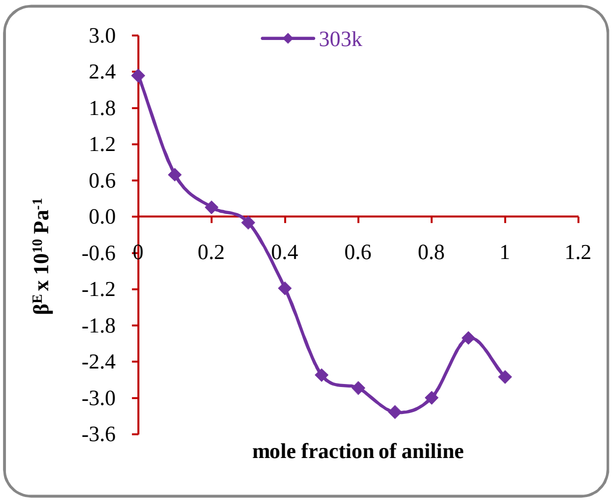

**Fig I** Mole fraction Vs. excess adiabatic compressibility

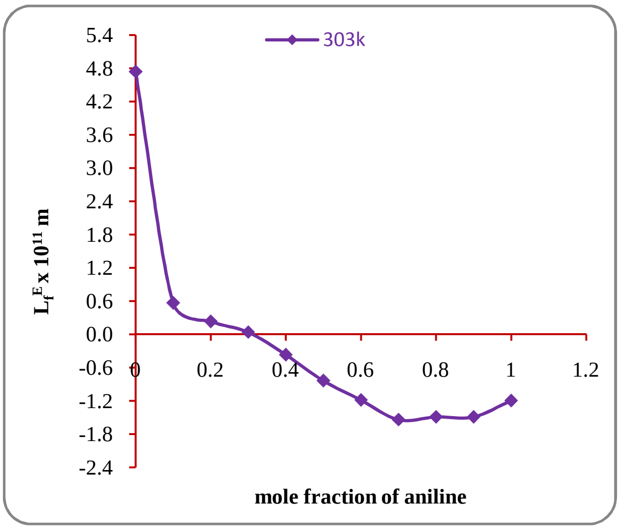

**Fig II** Mole fraction Vs. excess Free length

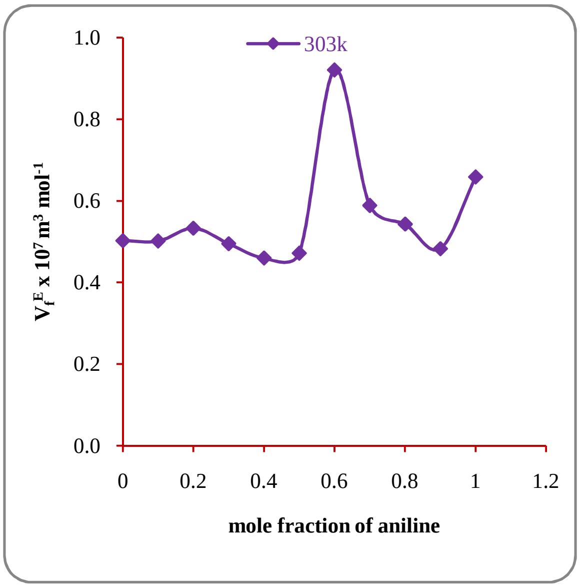

**Fig III** Mole fraction Vs. excess Free volume

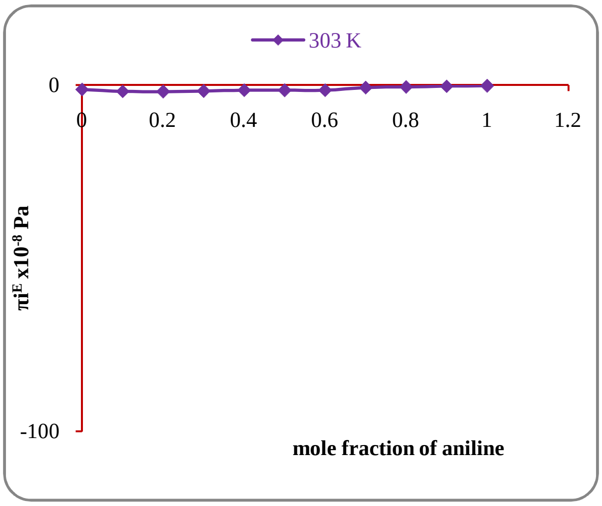

**Fig IV** Mole fraction vs. excess internal pressure

To comprehend the exact type of interaction prevails between the components, respective excess parameters have been calculated and for the present system, the perusal of Table III assumes Fig.1 to 4 the excess values are negative over the absolute mole fraction range. The excess adiabatic compressibility ($\beta^E$), free length ($L_f^E$) and internal pressure ($\pi_i^E$) are also initially positive and its goes to negative whereas both are acting in a similar manner (Thiyagarajan *et al*, 2008; Palaniappan *et al*, 2003). This distinctly confirms that the maximum number of component molecules get into complexation at this mole fraction.

## CONCLUSION

Presence of specific interaction is confirmed in the system. Aniline is found to readily influence the component molecules with its donor and acceptor groups. Weak dispersive and dipole-induced dipole type interactions are originated in the system. The observed excess negative parameters indicate their strong molecular interaction between unlike molecules.

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