Acoustic Investigation of the Self-Association of Aniline in 1-Hexanol-Hexane Mixtures At 303k

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Abstract: The study of ultrasonic velocities (u), densities (ρ), viscosities (η), were carried out for Aniline+1-Hexanol+Hexane at 303k. These ternary system was comprised of a polar, non-polar molecules and calculated thermo dynamical properties such as adiabatic compressibility (βa), free length (Lf), free volume (Vf), internal pressure (πi), and excess values predicted to the system. The results were combined with excess adiabatic compressibility reported previously to obtain ideal isothermal compressibility (KidT), ideal isobaric expansibility (αPid), and ideal molar heat capacitance (σid) derivatives of excess adiabatic compressibility (βE). These discusses the nature and strength of molecular intermolecular interaction in the system.

Keywords: Sound Velocity, Density, Molecular Interaction, Excess values.

I. Introduction

A previous in the study of liquid mixture, it was comprehended that the extent to which real liquid mixtures deviate from ideality is best expressed through the use of thermodynamics excess function (1-2). Excess properties of liquid mixtures reveal the existence of molecular interaction (3-4). In many petrochemical industrialized application, liquid mixtures rather than single component liquid system, are used in processing and product formulation (4-5). The present ultrasonic investigation deals with density, viscosity, velocity computation of adiabatic compressibility and its excess values at 303k in the ternary system of Aniline+1-Hexanol+Hexane.

II. Experimental details

The liquid combinations of various concentrations in mole fraction were prepared by taking AR grade chemicals, which were decontaminate by standard methods (6). The ultrasonic velocity (U) in liquid mixtures have been deliberated using an ultrasonic interferometer (Mittal type, Model F-80) working at 2 MHz 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 10⁵ for density and 0.001 Nsm⁻² for viscosity.

Using the deliberated data, the acoustical restrictions such as adiabatic compressibility (βa_C), free length (L_f), free volume (V_f), and internal pressure (πi) and their excess restrictions have been enumerated using the following standard expressions (7).

\[ \beta = \left( \frac{U^2 \rho}{2\eta} \right)^{\frac{3}{2}} \]  
\[ L_f = K_T \beta^{\frac{1}{2}} \]  
\[ V_f = \left[ \frac{M_{eff} U}{\eta k} \right]^{\frac{3}{2}} \]  
\[ \pi_i = bRT \left[ \frac{k\eta}{U} \right]^{\frac{3}{2}} \left[ \frac{\rho^{\frac{2}{3}}}{M_{eff}^{\frac{7}{6}}} \right] \]  
\[ A^E = A_{exp} - A_{id} \]

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\[ A_{id} = \sum x_i A_i \]  
\[ \beta = 1/\rho U^2 \]  
\[ \beta_E = \beta_{exp} - \beta_{id} \]  
\[ K_T^{id} = \sum \phi_i K_{T,i} \]  
\[ \alpha_p^{id} = \sum \phi_i \alpha_{p,i} \]  
\[ \sigma^{id} = \sum \phi_i \sigma_i \]  
\[ \sigma = C_{p,m}/V_m \]  
\[ \phi_1 = (X_1 V_1)/\sum (X_i V_i) b \]  

As \( \rho \) increases, the number of particles in a given region is increased and this leads to quick transfer of sound energy and thus velocity also increases (15-16). As aniline having a high boiling point, the energy between molecules of aniline is so high that the molecular bonds of aniline cannot be ruptured, whereas for 1-hexanol, it is not so. The increasing mole fraction aniline supports rupturing of components and hence, increase in viscosity (17) is expected. All the observed values vary linearly and this indicates the existence of interaction in the medium. This is in line with the observation made in some ternary system.
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Table 2. Values of adiabatic compressibility ($\beta_a$), free length ($L_f$), free volume ($V_f$) and internal pressure ($\pi_i$) of Aniline+1-Hexanol+Hexane at 303k.

<table>
<thead>
<tr>
<th>Mole Fraction</th>
<th>$\beta_a \times 10^{10}$Pa$^{-1}$</th>
<th>$L_f \times 10^4$m</th>
<th>$V_f \times 10^4$m$^3$mol$^{-1}$</th>
<th>$\pi_i \times 10^8$Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>X_t X_h X_3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0000</td>
<td>0.7000</td>
<td>7.8973</td>
<td>5.6519</td>
<td>1.4285</td>
</tr>
<tr>
<td>0.0771</td>
<td>0.2307</td>
<td>7.0655</td>
<td>5.3459</td>
<td>1.4564</td>
</tr>
<tr>
<td>0.2467</td>
<td>0.2460</td>
<td>5.8909</td>
<td>4.8814</td>
<td>1.1728</td>
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<tr>
<td>0.4552</td>
<td>0.2145</td>
<td>5.4426</td>
<td>4.6920</td>
<td>1.0504</td>
</tr>
<tr>
<td>0.6586</td>
<td>0.2304</td>
<td>4.7341</td>
<td>4.3748</td>
<td>0.7705</td>
</tr>
<tr>
<td>0.5362</td>
<td>0.2291</td>
<td>4.4401</td>
<td>4.2379</td>
<td>0.6799</td>
</tr>
<tr>
<td>0.6197</td>
<td>0.2306</td>
<td>3.8137</td>
<td>5.9276</td>
<td>0.6008</td>
</tr>
<tr>
<td>0.7000</td>
<td>0.0000</td>
<td>3.6760</td>
<td>5.8560</td>
<td>0.5697</td>
</tr>
</tbody>
</table>

The calculated values of $\beta_a$, $L_f$, $V_f$, and $\pi_i$ for the present system are given Table 2. As expected $\beta_a$ and $V_f$ are continuously decreasing with increasing mole fraction of aniline [18]. The inspection of these trends reveals a unanimous higher $\beta_a$ (and $V_f$) which reveals that the present system can provide some compactness, and the observed trend of $L_f$ confirms the existence of strong dipolar type interaction is evident.

The $V_f$ and $\pi_i$ values are behaving mutually opposite to each other. Decreasing $V_f$ and increasing $\pi_i$ values with increasing mole fraction of aniline is noticed, as observed in other liquid system [19]. Further, the gradual increase in $\pi_i$ indicates that the adhesive forces between the components are much more enhanced than the cohesive forces within the component. All the observation fully supports the existence of dipolar type interaction, especially at higher mole fraction aniline. To confirm the existence of interaction in system, it’s to calculate the excess values of the parameter considered in the work.

The excess parameters have been calculated and are illustrated in figures 1-4. The values for ternary mixture are $\beta_a^E$ and $L_f^E$ shows a continuous increase in magnitude and confirms that the strong interaction are enhanced as aniline mole fraction is increased. The trends of $V_f^E$ and $\pi_i^E$ are initial trends negative and exhibit a dip at 0.3 mole fraction of aniline. Further, a more or less symmetrical variation is noticed on either side of the dip in both $V_f^E$ and $\pi_i^E$ values[20]. The observation support that all the added aniline are in the cluster formation with hexane+1-hexanol binary complexes at this mole fraction.
V. Conclusions

i) The presence of specific strong dipolar interaction is in the ternary system.

ii) A weak dispersive interaction in small magnitude exists at lower mole fraction.

iii) All the component molecules get completely engaged in the interaction process.

References

[6]. C V. Suryanarayana, Indian J. Chem. 10 (1972) 713.