

Molecular Interaction Studied of Binary Liquid Solutions of isoamyl alcohol and isobutyl alcohol in benzyl amine

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ABSTRACT

Viscosity(η), Density(ρ) and Ultrasonic velocities(U) are reported for binary mixtures of isoamyl alcohol and isobutyl alcohol with benzyl amine over entered range of mole fractions at 303.15 and 313.15 K and atmospheric pressure. The viscosity deviation ($\Delta\eta$) Excess molar volume (V_E) and isentropic compressibility (K_s) have been calculated. These values were fitted with Redlich-Kister type polynomial equation.

Keywords : Viscosity, Density, Ultrasonic velocities, Redlich-Kister.

I. INTRODUCTION

The Viscosity (η), Density (ρ) and Ultrasonic velocities (U) measurements find wide applications in characterizing the physico-chemical behavior of liquid mixtures and in the study of molecular interactions¹⁻³. The measurements of Ultrasonic velocity of a liquid and mixtures allows the calculations of compressibility and hence enables to obtain structural information⁴, In turn the data of sound velocity can be subjected to scrutiny by applying Jacobins free length and schaafts collision factor theory. The deviations observed in free length and other parameters have been attributed to dipole-dipole, dipole-induced dipole and other dispersive force interactions⁵⁻⁷. It is well known that aqueous solutions of hydrocarbons, alcohols, amines, ethers are characterized by H-bonding and hydrophobic interactions. The investigations regarding the molecular association in organic binary mixtures having alkanol group as one of the component is of particular interest, since alkanol group is highly polar and can associate with any other group having some degree of polar attractions. benzylamine is protic,

strongly associated due to highly polar $-NH_2$ group in the molecule and has large dipole moment¹⁴.

In view of the importance mentioned, an attempt has been made to elucidate the molecular interactions in the mixtures of benzylamine with branched alkanols (C_5 & C_4) at all compositions and four temperatures. In this article only the data of binary mixtures of benzyl amine with isoamyl alcohol and isobutyl alcohol respectively at *303.15 and 313.15 K* is reported.

II. METHODS AND MATERIAL

A. Experimental:

All the chemicals used in the present research work are analytical reagent (AR) and spectroscopic reagent (SR) grades of minimum assay of 99.9% obtained from E-Merck, Germany and Sd Fine chemicals, India, which are used as such without further purification. The purities of the above chemicals were checked by density determination at *303.15 and 313.15 K* the uncertainty is less than $\pm 1 \times 10^{-4} \text{ g cm}^{-3}$. The binary liquid mixtures of different known

compositions were prepared in stopper measuring flasks. The density, viscosity and velocity were measured as a function of composition of the binary liquid mixture of benzyl amine with isoamyl alcohol and isobutyl alcohol respectively at 303.15 and 313.15 K. The density was determined using a Bi-capillary pycnometer. The weight of the sample was measured using electronic digital balance with an accuracy of ± 0.1 mg (Model: Shimadzu AX-200). An Ubbelohde viscometer (20ml) was used for the viscosity measurement and efflux time was determined using a digital clock to within ±0.01s. An ultrasonic interferometer having the frequency of 2 MHz (Mittal Enterprises, New Delhi, Model: F-81) with an overall accuracy of ± 0.1% has been used for velocity measurement. An electronically digital operated constant temperature bath (RAAGA Industries) has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature with an accuracy of ± 0.01 K.

B. Theory and Calculations

Excess volumes of the mixtures have been calculated using density and mole fraction data given by equation:

$$V^E = (M_1X_1+M_2X_2)/\rho_{12} - (M_1X_1)/\rho_1 - (M_2X_2)/\rho_2 \quad --(1)$$

Viscosity of Binary Mixtures is calculated by:

$$\ln \eta_m = X_1 \ln \eta_1 + X_2 \ln \eta_2 \quad --(2)$$

The measured viscosities of the mixtures have been used to obtain deviation in Viscosity parameters on the basis of linearity in following way,

Deviation in Viscosity of Binary Mixtures is calculated by :

$$\Delta \eta_m = \eta_{12} - X_1 \eta_1 - X_2 \eta_2 \quad --(3)$$

Deviation in isentropic compressibility have been evaluated by using the equation

$$\Delta k_s = k_s - (\Phi_1 k_{s1} + \Phi_2 k_{s2}) \quad --(4)$$

where k_{s1} , k_{s2} and K_s are isentropic compressibility of liquid mixtures and Φ is volume fraction of pure i^{th} component in the mixture and is defined as

$$\phi = (x_i V_i) / (\sum x_i V_i)$$

where x_1 and V_i are mole fraction and molar volume of i^{th} component in the mixture

The excess properties y^E are fitted by the method of non linear least squares to a Redlich kister type polynomial (5)

$$y^E = X_1 X_2 \sum A_i (X_1 - X_2)^i \quad --(5)$$

In each case the optimum number of coefficients A_i was determined from an examination of the variation of standard deviation as calculated by :

$$\sigma y^E = [\sum (y^{E_{obs}} - y^{E_{cal}})^2 / (n-m)]^{1/2} \quad --(6)$$

where n represents the number of experimental points and m represents the number of coefficients in fitting the data.

$$Z^E = Z_{mix} - x_1 Z_1 - x_2 Z_2 \quad --(7)$$

$$L_f^E = L_{fmix} - x_1 L_{f1} - x_2 L_{f2} \quad --(8)$$

Various physical and thermo dynamical parameters are calculated from the measured data such as

Adiabatic Compressibility

$$\beta_s = 1 / (U^2 \rho) \quad --(9)$$

Intermolecular free length

$$L_f = K \sqrt{\beta} \quad --(10)$$

where K is a temperature dependent constant.

Free volume

$$V_f = (M_{ef} U / K \eta)^{3/2} \quad --(11)$$

where M_{ef} is the effective molecular weight ($= m M_x$, in which m and x are the molecular weight and the mole fraction of the individual constituents respectively). K is a temperature for all liquids.

Available volume

$$V_a = V T (1 - U / U) \quad --(12)$$

where U is the limiting velocity and is taken as 1600 ms and V is the molar volume at T_K .

Excess values of the above parameters can be determined using

$$A^E = A_{exp} - A_{id} \quad --(13)$$

where $A_{id} = \sum A_i X_i$, A_i is any acoustical parameters and X_i the mole fraction of the liquid component.

In this content, the excess properties like excess volume, excess partial volume, excess free energies and entropies have been found useful in characterizing the molecular interactions. Alcohols are linear H-bonded liquids, have been studied in detail, they show aggregation in non polar solvents like CCl_4 ⁵. In this we thought on the problem that the self-association of alcohol molecules can be detected in polar solvents like benzyl amine. It has been examined by studying the excess volume, excess viscosity and other parameters. The results and other details are given below.

III. RESULTS AND DISCUSSION

The experimental values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations ($\Delta\eta$) and deviation on isentropic compressibility (ΔK_s) for the two binary liquid systems at 303.15 and 313.15 K, are given in Tables 1 and 2. The variation of excess parameters with the mole fraction of alkanols (x_2) at 303.15 and 313.15 K are plotted in Fig.1-8.

The measured parameters viz. density (ρ) viscosity (η) ultrasonic velocity (U) and calculated parameters such as adiabatic compressibility (K_s), intermolecular free length (L_f) and volume fractions (Φ) for the System 1 : isoamyl alcohol (1) + benzyl amine (2) at 298.15 K are given in Table 1 and 2, for the System 2 : isobutyl alcohol (1) + benzyl amine (2) at 303.15 and 313.15 K are given in Table 1 and 2.

It is evident from the Table 1 and Table 3, that both the systems (I) and (II), ultrasonic velocity increases with increase in concentration of benzyl amine (2). This indicates that, strong interaction observed at lower concentration of alcohols. The density values also have the same trends with velocity in the systems (I) and (II). Density increases due to the

increased electrostriction in that solution. This more electrostriction decreases the volume and hence increases the density. Viscosity decreases in systems I and II with increase in benzyl amine, suggesting there by more association between solute and solvent molecules.

The adiabatic compressibility (K_s) increases with increase in the concentrations of isoamyl alcohol / isobutyl alcohol in benzyl amine (2). This is due to increase in structural disorder of benzyl amine resulting in less cohesion, and leads to a increase in K_s . The increase in K_s results in an decrease in the value of U.

The parameter, the free length (L_f) is calculated from the ultrasonic velocity (U) and adiabatic compressibility (K_s). It is observed that L_f , increases with the concentration of isoamyl alcohol / isobutyl alcohol in benzyl amine (2). Increase in intermolecular free length leads to negative deviation in sound velocity and positive deviation in compressibility. This indicates that the molecules are away from each other in the both system.

Values of G^E are more negative at lower temperature provides additional evidence for the existence of interactions of weak magnitude like dipole-induced dipole type between components of liquid mixtures¹². The magnitudes of G^E for isoamyl alcohol are slight positive than that of isobutyl alcohol at both temperatures.

In their pure state, the self association of alkanols decreases with increasing chain length, when alkanols are mixed with benzyl amine then there is interaction between their individual functional groups (-OH and -NH₂). The presence of electron withdrawing group on benzene ring decreases its electron densitie^{8,9}

The curves for V^E , $\Delta\eta$, Δk_s and G^E values are plotted against mole fractions of alkanols, these curves are negative over the most mole fraction of the alkanols at 303.15 and 313.15 K (Fig.1-8). These curves are U-shaped with minima around $x_1 = 0.4-0.5$ mole fraction of the alkanol. These excess parameters at a particular mole fraction of the alkanols becomes less negative with increase of temperature. The negative values may be attributed to the existence of dispersion and dipolar forces between unlike molecules and related to the difference in size and shape of the molecules^{10,11}. The V^E values are negative at lower temp. as decrease in temperature disturb hereto and homo-association of the molecules which causes decrease in fluidity of the liquid. The V^E values are positive at 313.15K. The magnitude of V^E , $\Delta\eta$, Δk_s , and G^E the sign and the extent of deviation of these properties from ideality depend on the strength of interaction between unlike molecules. The excess viscosity gives the strength of the molecular interaction between the interacting molecules. For systems where dispersion, induction and dipolar forces which are operated by the values of above excess parameters are found to be negative, the large negative values of excess viscosity for all the systems can be attributed to the presence of the dispersion, induction, and dipolar forces between the components. The magnitude of V^E , $\Delta\eta$ and Δk_s are more at higher temperature provides inverse relation with G^E

IV. CONCLUSION

The present investigation shows that greater molecular interaction exists in isobutyl alcohol mixtures which may be due to hydrogen bond formation and weak molecular interaction that exists in the isoamyl alcohol mixtures and which may be due to the dominance of dispersion forces and dipolar interaction between the unlike molecules¹². The V^E values are positive at 313.15K as the interaction tends to be weaker with rise in temperature which may due

to weak intermolecular forces and thermal dispersion forces^{13,14}. The existence of molecular interaction in the mixture is in the order: isobutyl alcohol > isoamyl alcohol

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V. REFERENCES

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