Analysing Dielectric and Ultrasonic Studies of Liquid Mixtures

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Abstract

The characteristics of liquid mixes are extremely relevant in thermodynamic, acoustic, and transport investigations. The compositional dependency of thermodynamic characteristics has shown to be a highly effective tool in understanding the type and extent of molecular aggregation caused by intermolecular interaction. This form of research is effective for characterising the many features of the physicochemical behaviour of liquid mixtures. Density, viscosity, and ultrasonic velocity (U) measurements were performed at 303, 308, and 313K for three ternary organic liquid mixes of 1-alkanols in binary mixtures of tetrahydrofuran (THF) and 1-chlorobutane (3:1) ratio. Acoustic characteristics such as adiabatic compressibility (β), free length (Lf), free volume (Vf), internal pressure (πi) and Gibb's free energy (ΔG) have been computed using experimental data. The excess values of the aforementioned parameters, as well as the Grunberg-Nissan interaction parameter (d), have also been assessed and discussed in light of molecular interaction in the mixes.

Keywords: *Liquid, Binary, Alcanols, Mixtures, Organic.*

I. INTRODUCTION

The type and degree of pattern molecule aggregations that exist in multi-component systems as a result of molecular interactions are revealed by ultrasonic measurements. The ultrasonic method is used to investigate the characteristics and structures of liquids, as well as the presence and intensity of molecular interactions between liquid components. The study of intermolecular interactions is vital in molecular sciences, and liquids, liquid mixes, and solutions have many uses in the chemical, textile, pharmaceutical, and nuclear industries. The infrared, Raman, and dielectric characteristics are also employed to examine molecule interactions. The ultrasonic velocity and density data for liquid mixes of alcohols with ketoneat 303.15K were used to investigate molecular interactions and forecast probable interactions between dissimilar molecules.

Dielectrics are a type of substance that becomes polarised when exposed to an electric field. These are electrically insulating materials that have an electric dipole moment permanently or briefly in the presence of an applied electric field. Electrical insulators are all dielectric materials, while dielectric materials are not all insulators. Dielectric materials are mostly utilized to store electrical energy as well as to act as electrical insulators. In general, they are non-metallic materials with a high specific resistance and a negative temperature coefficient. Though these materials lack free charge carriers for conduction, they do contain positive and negative charges that are bonded together and may be impacted by the applied electric fields.

II. EXPERIMENTAL

All of the chemicals utilised in this study are spectroscopic reagent (SR) and analytical reagent (AR) grades with a minimum assay of 99.9 percent purchased from E-Merck, Germany, and Sd Fine Chemicals, India, and are used as is. The purity of the aforementioned substances was determined by density determination at 303, 308, and 313K ± 0.1K, with an accuracy of ±1×10–4g on an electronic digital balance (Model: SHIMADZU AX 200). In stopper measuring flasks, ternary liquid mixes of various known compositions were created. The density, viscosity, and velocity of ternary liquid mixtures were determined as a function of composition at 303, 308, and 313K when 1-propanol, 1-butanol, and 1-pentanol were added to binary mixes of THF and 1-

chlorobutane. Binaries with preset mole ratios X1/X2 @ 3:1 were mass-produced for this purpose. The density was calculated with an accuracy of ±0.01 kg×m–3 using a specific gravity bottle and a relative measuring technique. The viscosity was measured using an Ostwald's Viscometer (10ml capacity), and the efflux time was estimated to within ±0.01s using a digital Chronometer. For velocity measurement, an ultrasonic interferometer with a frequency of 3MHz (MITTAL ENTERPRISES, NEW DELHI, MODEL F-81) and an overall accuracy of 0.1 percent was utilised. To circulate water through the double-walled steel measuring cell carrying the experimental solution at the required temperature, an electrically digitally controlled constant temperature bath (RAAGA Industries) was employed. The temperature reading is accurate to ±0.1 K.

III. RESULTS AND DISCUSSION

The density (ρ), viscosity (η), and ultrasonic velocity (U) experimental values for pure liquids and three ternary liquid systems at 303, 308, and 313K. Tables show the excess values of viscosity, adiabatic compressibility, free length, free volume, internal pressure, Gibb's free energy, and the Grunberg interaction parameter 'd.' Excess acoustical parameters are presented in Figs.1-6 as a function of mole fraction of 1-alkanols (X3) in THF and 1-chlorobutane mixtures at 303, 308, and 313K, with curves constructed using least square fitting.

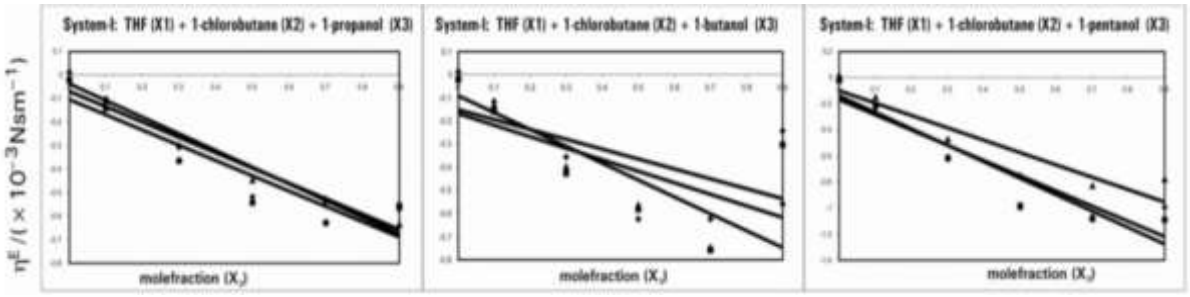

Figure 1: The variation of excess viscosity with molefraction of -alkanols in tetrahydrofuran and -chlorobutane mixture at 303, 308 and 313 K

The thermodynamic excess characteristics of liquid mixes are found to be more sensitive to intermolecular interactions between the component components. The sign and magnitude of excess parameter deviation are determined by the degree of contact between dissimilar molecules. In the study of intermolecular interaction, the measurement of viscosity in ternary liquid mixtures provides some accurate information. The excess viscosity, according to Fort et al., indicates the degree of the molecular contact between the interacting molecules. Excess viscosity is shown to be negative in systems where dispersion, induction, and dipolar forces are acting, but the presence of particular interactions leading to the creation of complexes in liquid mixtures tends to make excess viscosity positive. In all three systems, the extra viscosity (Fig.1) is negative across the entire concentration range. According to the study and careful observation, they decrease as the concentration of 1-alkanols (X3) increases, but they grow non-linearly when the temperature rises. The observed behaviour of ηEin all systems suggests the less strengthening of interaction between the components of mixture.

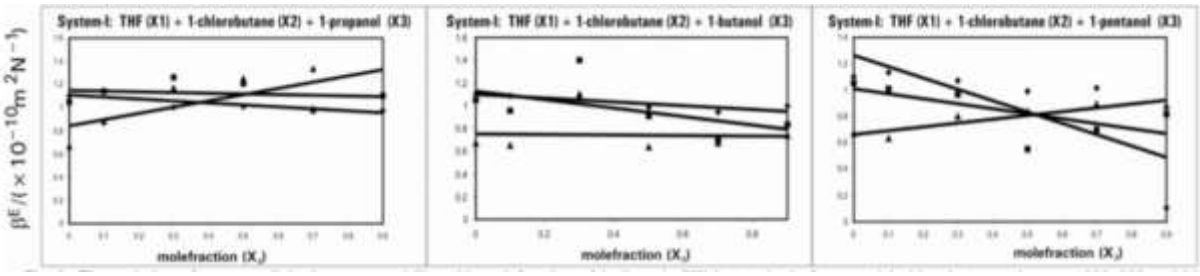

Figure 2: The variation of excess adiabatic copressbility with molefraction of 1-alkanols in tetrahydrofuran and 1-chlorobutane mixture at 303, 308 and 313 K

The Fig.2. shows that the excess value of adiabatic compressibilitiesare positive and it decreases non- linearly with increasing the concentration of X3 as well as rising of temperature in all systems studied. Fort et.al., found that the increasing negative value of excess compressibilites indicates greater interaction between the components of the mixtures. Positive values in excess properties correspond mainly to the existence of dispersive forces. The negative value of βEis associated with a structure forming tendency while a positive value is taken to indicate a structure breaking tendency due to hetero- molecular interaction between the component molecules of the mixtures. The negative βEvalues for ternary mixtures indicate, the formation of H bonds. The positive excess adiabatic compressibility which indicates loosely packed molecules in the mixtures results due to shape and size. In the present investigation, the positive contribution of βEin all systems suggests the existence of dispersive forces, and the decreasing behaviour of βEvalues with increasing of 1-alkanols as well as rise in temperature shows the weakening of interaction exists in the mixtures.

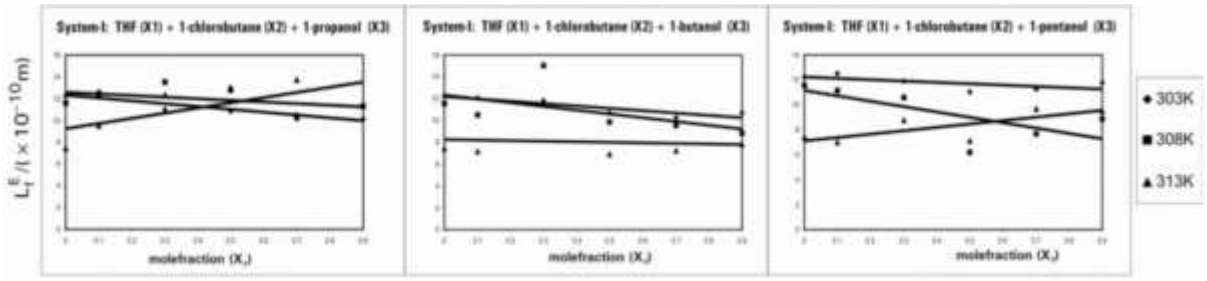

Figure 3: The variation of excess freelength with molefraction of 1-alkanols in tetrahydrofuran and 1-chlorobutane mixture at 303, 308 and 313 K

Excess free length varies positively and decreases non-linearly with increasing 1-alkanol concentration and rising temperature in all systems examined, as shown in Fig.3. According to Ramamoorthy et al., negative values of excess intermolecular free length show that sound waves span greater distances due to a drop in intermolecular free length, implying that hydrogen bond interaction between dissimilar molecules is dominating. According to Fort et al., positive excess free length values should be assigned to dispersive forces, whereas negative excess free length values should be attributed to charge transfer, dipole-induced dipole, and dipole-dipole interactions. The presence of dispersive forces between the components of the mixes is demonstrated by the positive contribution of LE in all systems in the current investigation. Spencer et al. made a similar observation based on excess free length values.

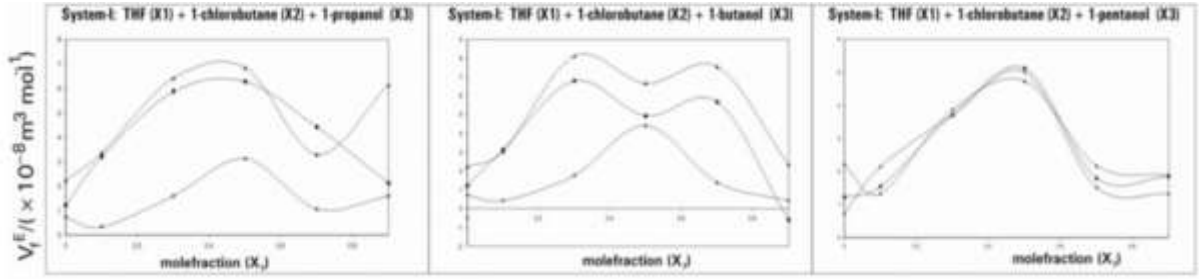

Figure 4: The variation of excess free volume with molefraction of 1-alkanols in tetrahydrofuran and 1-chlorobutane mixture at 303, 308 and 313 K

Figure 4 depicts the surplus free volume for ternary liquid combinations in a qualitative manner. The values of LEF are discovered to be positive and grow with increasing the molefraction of X3 up to 0.5, after which they drop for all mixes. Furthermore, in all systems tested, these values rise as the temperature rises. Fort et al. observe that for various ternary liquid combinations, the negative excess free volume tends to diminish as the intensity of the contact between the unlike molecules grows, despite the fact that this does not parallel with the excess compressibility. VE values are the sum of contributions from a number of opposing effects. These may be arbitrarily separated into three types: chemical, physical, and structural contributions. Physical contributions,

which are non-specific interactions between the genuine species in the mixture, add a positive term to VE. Negative value VE is contributed by chemical or particular intermolecular interactions, as well as structural (interstitial accommodation). The presence of dispersive interactions between the component molecules of the mixes is demonstrated by the positive contribution of VE in all systems in the current investigation. Furthermore, the observed behaviour of VE with increasing temperature indicates that the intensity of contact weakens in all systems tested. The magnitude of VE values is as follows: 1-butanol > 1-propanol > 1-pentanol.

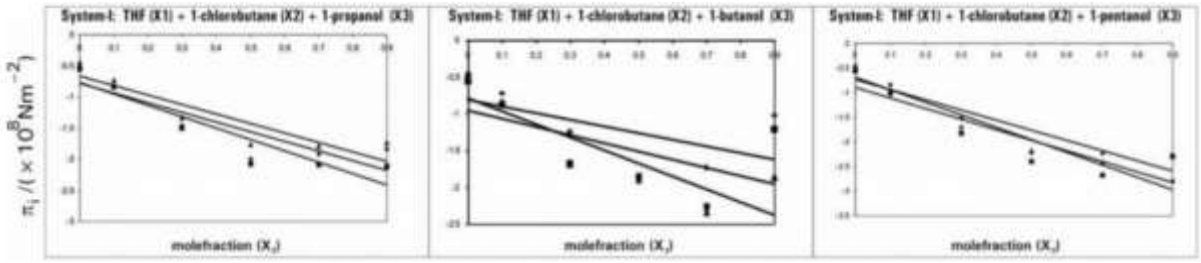

Figure 5: The variation of internal pressure with molefraction of 1-alkanols in tetrahydrofuran and 1-chlorobutane mixture at 303, 308 and 313 K

In the study of ternary liquid mixtures, the variation of the internal pressure may give some information regarding the nature and strength of the forces existing between the molecules. The excess internal pressure values (Fig.5) is found to be negative and it decreases with increasing the molefraction of (X3) aswell as temperature in all the three systems studied. The negative values ofE indicates that onlydispersion and dipolar forces are operating with complete absence of specific interaction. In the presentinvestigation, the observed behaviour ofshows the existence of dispersive forces in all systemsstudied, but the strength of interaction decreases with rising of temperature results the decreasing of p Evalues.

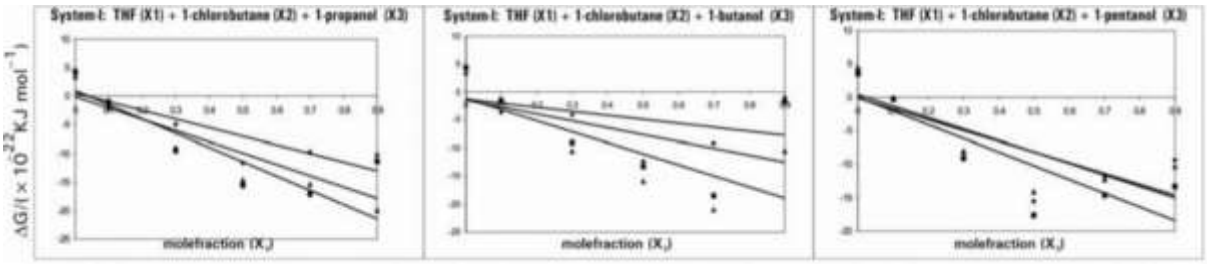

Figure 6: The variation of Gibb's free energy with molefraction of 1-alkanols in tetrahydrofuran and 1-chlorobutane mixture at 303, 308 and 313 K

Fig.6 shows the variation of excess Gibb's free energy is found to be negative in all systems studied and it decreases with increasing the mole fraction of (X3) as well as with elevation of temperature. According toReed et.al., the positive deviation inΔG^E may be attributed to specific interactions like hydrogenbonding and charge transfer, whereas the negative deviations may be ascribed to dispersion forces with systems. In the present investigation, the negative excess Gibb's free energy (ΔG^E) obtained in all the systems shows the dominance of dispersion forces. Recently, Ali et.al., attributes the increasing positive values of ΔG^E in few ternary liquid mixtures, to hydrogen bond formation between unlike molecules.

The interaction parameters 'd' in the Grunberg and Nissan equation represents the intensity of the interaction between the mixing components. The results demonstrate that the values of 'd' become negative and drop as the quantity of 1-alkanols increases as well as the temperature rises in all three systems tested. The following 'd' numbers were said to signify different forms of interactions. Big and positive 'd' values imply strong particular interaction, whereas tiny positive values suggest weak specific interaction and large negative values indicate no specific interaction. The dominance of dispersion forces can be attributed to negative values of 'd.' resulting from the breakage of hydrogen bonds in the related component of the mixes, according to Kalara et al. In the

current study, negative values of 'd' in ternary systems were attributed to the absence of particular interactions between dissimilar molecules. Furthermore, the decreasing behaviour of 'd' values with increasing temperature indicates a decrease of interaction between mixture components.

IV. CONCLUSION

The ultrasonic technique is a potent probe for determining the physico-chemical characteristics of a mixture and the presence of molecular interaction. The density, viscosity, and computed excess acoustical characteristics also give proof of validation. The presence of weak molecular connection between the mixing components is inferred from the excess acoustical parameters, which might be attributed to the dominance of dispersion and dipolar forces. Furthermore, due to weak intermolecular interactions and thermal dispersion forces, the intensity of interaction weakens as temperature rises.

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