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Molecular Interaction Study through Free Length and Available Volume For Ternary Liquid Mixture of Alcohol + Tea + Acetic Acid

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Abstract: ***The ultrasonic wave propagation through medium of binary and ternary liquid mixture has been drawing a special attention of physicists because of their peculiar behaviour and wide applications in biomedical science. The ultrasonic velocity and related acoustical parameters are the important tools in understanding the nature of intermolecular interactions between components of liquid mixture. The density, ultrasonic velocity and viscosity at three different temperatures 303K, 308K, and 313 K have been measured in the ternary systems of Alcohol + Tri-ethyl amine(TEA)+ Acetic Acid. The ultrasonic velocity measurements were made at 3 MHz by using ultrasonic interferometer. The free length and available volume have been calculated for ternary liquid mixtures. The dependence of ultrasonic speed and other derived parameters is indicative of the presence of molecular interactions. The experimental findings are used to interpret the nature of inter molecular interactions.***

Keywords: Molecular interaction, Available Volume, Free length, Ultrasonic velocity, ternary liquid mixture.

1. Introduction

Now-a-days ultrasonic is an area of intense scientific and technological research. In view of its extensive scientific and engineering applications it has attracted attention of researchers, non-destructive testing professionals, industrialists, technologists, medical practitioners, instrumentation engineers, software engineers and medical scientists. The acoustic and thermodynamic properties have been used to understand the different kinds of interactions and their strengths. The nature and degree of molecular interactions in different solutions changes depending upon the nature of solvent, the structure of solute molecule and extent of solution taking place in the solution [1-4]. Knowledge of variation of velocity with concentration provides vital information about molecular interaction. Adiabatic compressibility (β) and intermolecular free length (L_f) are the function of ultrasonic velocity. Liquid mixtures consisting of polar and non-polar components are of immense importance. When two or more liquids are mixed, there occur some changes in physical and thermodynamic properties because of free volume change, change in energy and change in molecular orientations. Here in the present study the ultrasonic velocity, density and viscosity measurements have been carried out at different concentrations and temperatures 303K, 308K, 313K for the determination of ultrasonic parameters such as molecular free length (L_f) and available volume.

2. Experimental Study

In the present study alcohol, acetic acid and TEA were obtained commercially of AR grade with purity of 99.5% and used without further purification. The chemicals used were obtained from Merch, (Mumbai). The ternary liquid mixture was prepared at room temperature. Samples were prepared by mixing the component liquids in volume proportion. Every time 28ml of solution was prepared for the measurement of density, viscosity and ultrasonic velocity. The ultrasonic velocity (U) in liquid mixture is measured using an ultrasonic interferometer (Mittal type, Model F-81) working at 3MHz frequency and at three different temperatures 303K, 308K and 313K. The accuracy of sound velocity was ±0.1 ms-1. An electronically operated digital constant temperature water bath has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature. The densities (ρ) of the system were measured on electronic balance with calibrated density bottle. Ostwald's viscometer was used for the viscosity measurement of pure liquids and liquid mixtures with an accuracy of ±0.0001NSm-2

3. Theory

The experimentally measured ultrasonic velocity (u) , density (ρ) and viscosity (η) are used to evaluate various thermo dynamical parameters like compressibility (β_a),

$\beta_a = 1/U^2 \rho$

Where ρ stands for density liquid and β_a is adiabatic compressibility.

Intermolecular free length(L_f),

$L_f = K\beta_a^{1/2}$, Where, K is temperature dependent constant

Available volume,

$Va_{mix} = V (1-u/u_\infty)$,

Where u is velocity, u_∞ is constant and its value is 1600m/s and V is molar volume.

4. Result and discussion

The measured ultrasonic velocity, density and viscosity of alcohol + TEA + Acetic acid are used for further calculation of acoustical parameters like adiabatic compressibility, free length and available volume at 303K, 308K and 313K. The measured parameters *viz*., ultrasonic velocity (U), calculated intermolecular free length (L_f) and Available volume for

system: alcohol + TEA + Acetic Acid at temperature 303K, 308K, 313K are given in table I, II, III. The plots of the free length

Table 1: Alcohol +TEA + Acetic Acid at 303K

Sr. No.	*Mole Fraction of TEA*	*Mole Fraction of Acetic Acid*	*Ultrasonic Velocity (U) m/sec*	*Free length (L_f) (A^0)*	*Available Volume (Va) Cm^3/mole*
1	0.2951	0.0000	1152	0.905292	47.6771
2	0.2385	0.0969	1194	0.841503	38.96861
3	0.1880	0.1834	1215	0.80969	34.50477
4	0.1427	0.2610	1569	0.764565	28.16303
5	0.1018	0.3309	1254	0.766028	28.21847
6	0.0647	0.3944	1221	0.786915	30.28908
7	0.0309	0.4523	1200	0.795726	30.96939
8	0.0000	0.5052	1155	0.824532	33.65999

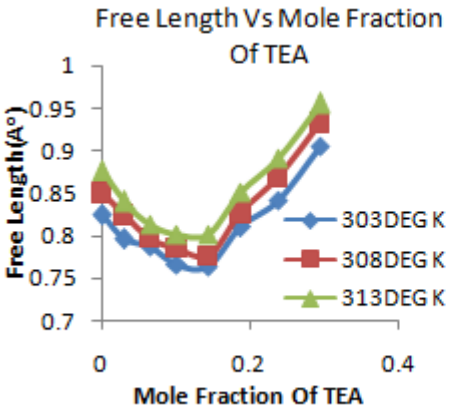
Table 2: Alcohol +TEA + Acetic Acid at 308K

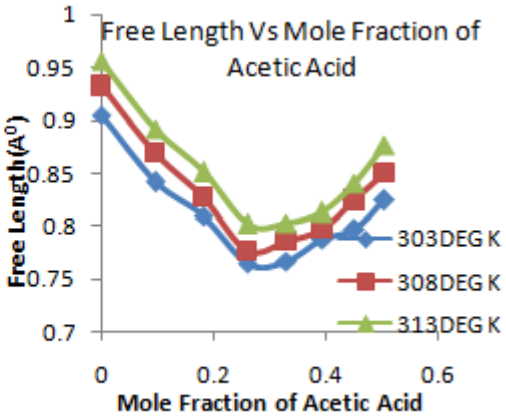
Sr. No.	*Mole Fraction of TEA*	*Mole Fraction of Acetic Acid*	*Ultrasonic Velocity (U)m/sec*	*Free length (L_f) (A^0)*	*Available Volume (V_a)Cm^3/mole*
1	0.2951	0.0000	1128	0.932524	50.30064
2	0.2385	0.0969	1176	0.868832	41.42536
3	0.1880	0.1834	1200	0.826744	35.88706
4	0.1427	0.2610	1260	0.776592	28.96338
5	0.1018	0.3309	1236	0.786078	29.8942
6	0.0647	0.3944	1215	0.797184	30.7776
7	0.0309	0.4523	1170	0.824138	33.41701
8	0.0000	0.5052	1131	0.849911	35.57657

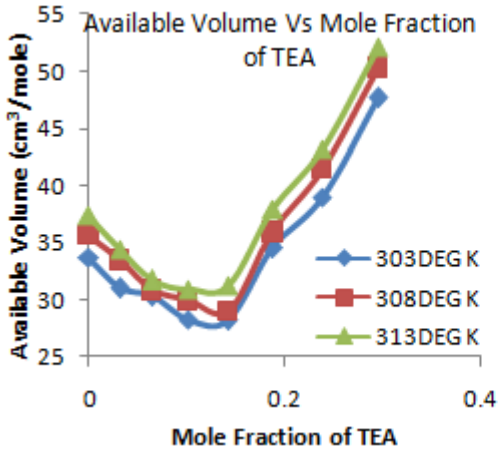
Table 3: Alcohol +TEA + Acetic Acid at Temp.313K

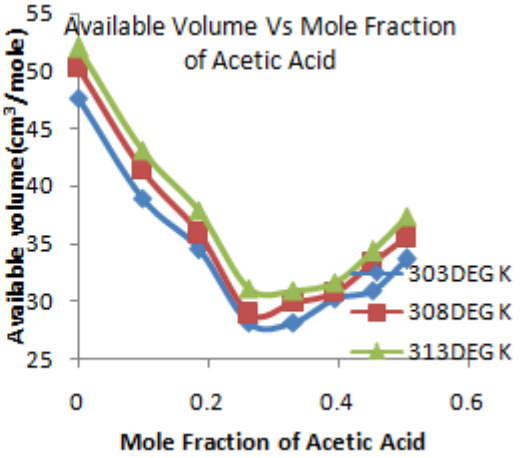
Sr. No.	*Mole Fraction of TEA*	*Mole Fraction of Acetic Acid*	*Ultrasonic Velocity (U) m/sec*	*Freelength (L_f) (A^0)*	*Available Volume (Va) Cm^3/mole*
1	0.2951	0.0000	1113	0.955868	52.10183
2	0.2385	0.0969	1161	0.891227	43.16811
3	0.1880	0.1834	1179	0.850989	37.91179
4	0.1427	0.2610	1236	0.801397	31.18324
5	0.1018	0.3309	1224	0.802079	30.94187
6	0.0647	0.3944	1206	0.813157	31.68752
7	0.0309	0.4523	1158	0.840565	34.35216
8	0.0000	0.5052	1110	0.876147	37.3387

versus mole fraction of at temperatures 303K, 308K, 313K are shown in graph I, II. The plots of available volume versus mole fraction at temperatures 303K, 308K, 313K is shown in graph III, IV. From graph I, II, III, IV it can be observed that the nature of overall variation of free length curves is nonlinear. Free Length is distance covered by molecule before collision. The value of free length decreases with concentration, becomes minimum and again increases with mole fraction of TEA that is, it shows concave nature .The value of free length L_f increases with temperature it concluded that there is significant interaction in liquid mixture[5]. The ultrasonic velocity should increase with decrease in free length as a result of strong interaction between the components[6]. Intermolecular free length (L_f) has an inverse relationship with ultrasonic velocity. Decrease in intermolecular free length in system leads to positive deviation in sound velocity[7]. This indicates that the molecules are closer in the system. Eyring and Kincard have proposed that free length is predominating factor in determining the variation of ultrasonic velocity of solutions[8].









The available volume is the space available for the molecule to move in an imaginary unit cell. This reduces internal pressure. It is seen in the present system that available volume changes with the composition of the system. As the concentration of TEA increases available volume decreases, at concentration 0.14 it becomes minimum and again increases. The available volume also shows the concave curve. The observed increased values of V_a in system are due to close association between solute and solvent.

5. Conclusion

In this work we have measured free length and available volume at three different temperatures 303K, 308K, 313K of different concentration of system Alcohol +TEA + Acetic acid. All the observations from the present study leads to conclude that the non linear variation of all the parameters measured for ternary liquid mixture indicates existence of interaction between the different molecules of the compounds in the mixture. For the observed molecular interaction, hydrogen bond formations are responsible for the interaction in the liquid mixture.

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