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Acoustical Studies on Molecular Interaction in Binary System at the Tempture 298K and Frequency 5MHz

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Abstract: ***An analysis of different thermodynamic properties as a function of temperature provides valuable information about their characteristics. The concentration and temperature dependence of acoustic and volumetric properties of multicomponent liquid mixtures has proved to be a useful indicator of the existence of significant effect resulting from intermolecular interactions. Moreover mixtures of different organic liquids and the solvents rather than single pure liquids are of great practical importance in most chemicals, industrial and biological processes as they provide a wide range of mixtures with desired properties. In continuation of our studies on molecular interactions in binary liquid mixtures here we report the result of the binary mixture of Acetonitrile (ACN) with methanol and ethanol. The densities (ρ), ultrasonic velocity (U) and viscosity (η) have been measure in binary liquids mixture of ACN with methanol and ethanol as a composition of 0.0 to 1.0 of ACN in methanol and ethanol. The results are analyzed and it has been observed that, weak dispersive type intermolecular interactions are confirmed in the system investigated. The nonlinear behavior of these parameters provides the knowledge about various interactions among the molecules.***

Keywords: Ultrasonic velocity, viscosity, density, acoustical parameters, molecular interactions, Acetonitrile, Methanol and Ethanol

1. Introduction

Ultrasonic study of liquids is a useful technique for understanding its physico-chemical properties of the liquid mixtures [1-3]. Ultrasonic measurements are extensively used to study the molecular interactions in pure liquids and liquid mixtures [4-7]. The study of properties of liquid mixtures consisting of polar as well as non - polar components has wide applications in industrial and technological processes [8-11]. Most of the work on binary mixtures is channelized towards the estimation of thermodynamic parameters like adiabatic compressibility, free length, free volume etc [12-15]. We report here the results of ultrasonic study of the binary mixtures, Acetonitrile + Ethanol and Acetonitrile + Methanol and covering the entire composition range at 298K and at the frequency 5MHz. A survey of the literature reveals that no ultrasonic measurements have been performed for above two binary mixtures. Having this in mind, in order to understand the molecular interactions between the participating components of the mixture, ultrasonic velocities (U), densities (ρ) and viscosity (η) were measured. Using the experimental ultrasonic velocity (U), densities (ρ) and viscosity (η), various thermodynamic parameters like adiabatic compressibility (βa), intermolecular free length (L_f), free volume (V_f) and internal pressure (π_i) were estimated. The thermodynamic parameters were used to interpret the molecular interactions taking place between the components of the binary mixtures.

2. Materials and Methods

The liquid mixtures of Acetonitrile + Ethanol and Acetonitrile + Methanol of various concentrations in mole fraction were prepared by taking AR grade chemicals. All the liquids used were further purified by standard procedure. The mixtures were preserved in well-stopper conical flasks. After the thorough mixing of the liquids, the flasks were left undisturbed to allow them to attain thermal equilibrium. In all the mixtures the mole fractions of Acetonitrile has been increased from 0 to1 in ethanol and methanol.

The ultrasonic velocities were measured by using a Multifrequency (1-10MHz) ultrasonic pulse interferometer (Model No. F-83, Mittal Enterprises, New Delhi). It consists of a high Multirange frequency generator (1 to 10MHz) and a measuring cell. The measurements of ultrasonic velocities were made at a fixed frequency of 5 MHz. Temperature was controlled by circulating water around the liquid cell from thermostatically controlled constant temperature water bath. The densities of pure liquids and liquid mixtures were measured by using a specific gravity bottle with an accuracy of ± 0.5%. For the viscosity measurement of pure liquids and liquid mixtures, an Ostwald's viscometer was used with an accuracy of ± 0.001 NSm^{-2}.

3. Results and Discussion

Using the experimental data of ultrasonic sound velocity (U), density (ρ) and viscosity (η), various acoustical parameters such as adiabatic compressibility (β_a), intermolecular free length (L_f), free volume (V_f), internal pressure (π_i) were calculated by the following equations (1-5).

$$\beta_a = (U^2\rho)^{-1} \quad \ldots\ldots (1)$$

$$L_f = K_T \beta a^{1/2} \quad \ldots.. (2)$$

$$V_f = (M_{eff}\, U/\eta K)^{3/2} \quad \ldots\ldots \quad (3)$$

$$\pi_i = bRT(K\eta/U)^{1/2}\,(\rho^{2/3}/M_{eff}^{7/6}) \quad \ldots\ldots (4)$$

Where K_T is the temperature dependent constant having a value $198.10*10^{-8}$ in MKS system at 298K, K is constant

equal to $4.28*10^9$ in MKS system, b is a cubical packing fraction taken as 2 for all the liquids, R is the Universal gas constant, T is the experimental temperature.

The experimentally determined values of density (ρ), viscosity (η), and ultrasonic velocity (U) at 298K for the system of Acetonitrile + Ethanol and Acetonitrile + Methanol were listed in Table-1. From these observed values, various acoustic parameters like adiabatic compressibility (βa), free length (L_f), free volume (V_f) and internal pressure (π_i) at the temperature 298K have been evaluated and were presented in the Table-2. The variation of βa, L_f, V_f, and π_i with mole fraction of Acetonitrile in Ethanol and Methanol at the temperature 298K were shown in Figures: I-IV. From the Table-1, it has been observed that the ultrasonic velocity and density increases with increasing the mole fraction of Acetonitrile in ethanol and methanol while the viscosity decreases. This may be due to association and dipole –dipole interaction between the component molecules. In the present systems, due to thermal agitation of component molecules, the inter-molecular interaction becomes weak and this is indicated by increase in ultrasonic velocity values. Table-2 and figs:-I-IV show the variation of adiabatic compressibility, free length, free volume, and internal pressure at 298K temperature and the concentration. From Table-2 and figures-I and II, it is observed that adiabatic compressibility and free length decreases with increase in the concentration of ACN in Ethanol and Methanol. The decrease in adiabatic compressibility indicates the enhancement of the bond strength. From Fig.:-III, it is also observed that the values of free volume increases with increase in molar concentration of ACN in Ethanol and Methanol. Fig:-IV show that, internal pressure decrease with increase in molar concentration of ACN in Ethanol and Methanol.

The variations of adiabatic compressibility (β_a), intermolecular free length (L_f), free volume (V_f), internal pressure (π_i) with respect to mole fraction (X) of Acetonitrile + Ethanol and Acetonitrile +Methanol binary systems are shown in Fig.:I, II,III and IV respectively

4. Tables and Figures

Table 1: Density (ρ), Velocity (U) &Viscosity (η) of Acetonitrile + Ethanol and Acetonitrile+ Methanol binary systems at 298K.

Mole fraction (X) of ACN	Density(Kg/m^3)		Velocity(m/s)		Viscosity(Ns/m^2)	
	Ethanol	Methanol	Ethanol	Methanol	Ethanol	Methanol
0.0	801.10	786.40	1130.00	1098.00	0.8850	0.5213
0.1	803.23	782.10	1139.10	1130.80	0.8239	0.5018
0.2	804.45	790.91	1146.00	1151.00	0.7830	0.4927
0.3	807.34	798.32	1158.33	1168.00	0.7249	0.4688
0.4	811.10	803.41	1169.00	1179.00	0.6721	0.4113
0.5	814.09	809.86	1176.67	1185.00	0.6089	0.3780
0.6	816.60	812.74	1192.20	1196.67	0.5503	0.3279
0.7	822.40	820.21	1211.10	1219.00	0.4958	0.2930
0.8	824.20	821.01	1226.00	1223.00	0.4263	0.2816
0.9	827.03	824.29	1232.00	1238.00	0.3641	0.2703
1.0	828.93	828.93	1246.00	1246.00	0.2750	0.2750

Table 2: Adiabatic compressibility (βa), free length (L_f), free volume (V_f) and internal pressure (π_i) of the binary systems Acetonitrile + Ethanol and Acetonitrile + Methanol at 298K.

Mole Fraction (X) of ACN	βa $*10^{-10}$ (Pa^{-1})		L_f $*10^{-10}$ (m)		V_f $*10^{-7}$ (m^3mol^{-1})		π_i $*10^8$(Pa)	
	Ethanol	Methanol	Ethanol	Methanol	Ethanol	Methanol	Ethanol	Methanol
0.0	9.7771	10.8630	0.6238	0.6521	00.299	00.626	13.90	10.06
0.1	9.5909	10.039	0.6178	0.6321	00.444	00.924	10.72	08.24
0.2	9.4491	09.5438	0.6133	0.6163	00.617	01.244	08.63	06.76
0.3	9.2367	09.1820	0.6063	0.6045	00.866	01.168	07.05	05.60
0.4	9.0244	08.9544	0.5993	0.5969	01.185	02.510	05.86	04.54
0.5	8.9039	08.7933	0.5953	0.5916	01.628	03.367	04.91	03.85
0.6	8.6292	08.5921	0.5860	0.5848	02.240	04.899	04.15	03.19
0.7	8.3218	08.2048	0.5755	0.5716	03.067	06.818	03.53	02.71
0.8	8.0819	08.4133	0.5672	0.5693	04.431	08.224	02.97	02.41
0.9	7.9830	07.9155	0.5637	0.5613	06.336	09.978	02.51	02.15
1.0	7.7704	07.7665	0.5561	0.5559	10.916	10.916	02.04	02.04

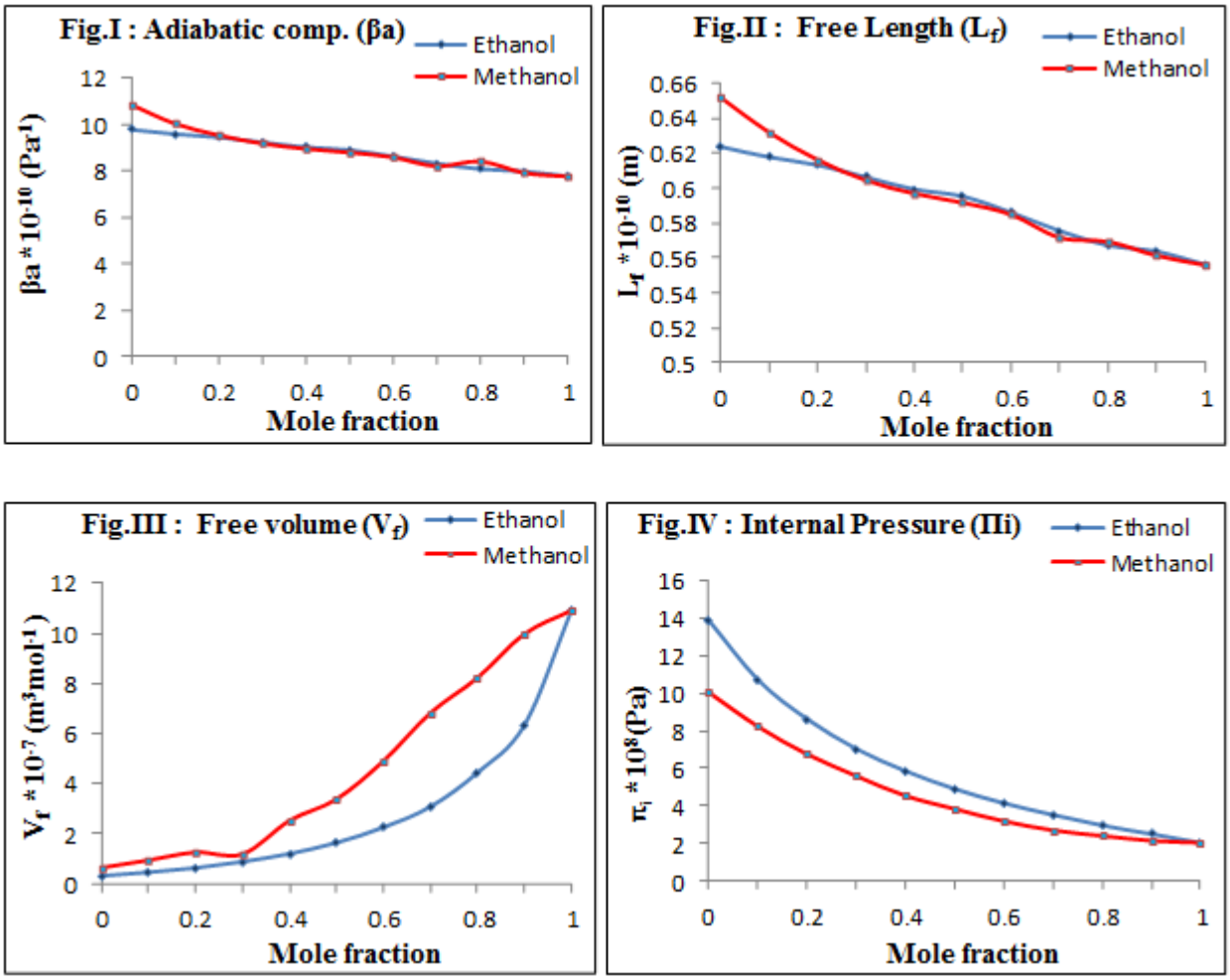

Figure I-IV: The variations of adiabatic compressibility (β_a), free length (L_f), free Volume (V_f), Internal pressure (π_i) w. r. to mole fraction (X) of the system: Acetonitrile + Ethanol and Acetonitrile + Methanol at 298K are shown in Fig.: I, II, III and IV respectively.

5. Conclusion

The observed increase of ultrasonic velocity indicates the solute-solvent interaction. The existence of solute-solvent type molecular interaction is favored in the system studied, confirmed from the U, ρ, η, βa, L_f, V_f and π_i data. The variation in ultrasonic velocity (U), density (ρ), viscosity (η) and other related thermodynamic parameters is non-linear. Ultrasonic velocity of the system increases, depending on the concentration of Acetonitrile. The non-linear behavior confirms the presence of solute-solvent, solvent-solvent, and dipole-dipole interactions. For the observed molecular interaction, hydrogen bond formations are responsible for the heteromolecular interaction in the liquid mixture. This provides useful information about inter and intra molecular interactions of the mixture as existing in the liquid systems.

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