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Ultrasonic studies of propanol-benzene, propanoal-methyl benzoate-benzene mixtures at 301 K

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ABSTRACT

The ultrasonic velocity, the density and viscosity have been measured for the binary and ternary mixtures containing propanol with benzene, propanol with methyl benzoate at 301 K over the whole range of concentration. From these values evaluated the adiabatic compressibility, free length, free volume, relaxation time, acoustic impedance, available volume, molar volume, Lenard John Potential, Rao constant and Wada's constant from the standard relations. Experimental and calculated values have been providing information regarding the nature of molecular interactions. These values are confirming the solute – solvent interaction for binary components and ternary components having strong interactions through hydrogen bonding.

Keywords: Propanol, methyl benzoate, benzene, Lenard John Potential, Hydrogen bonding,

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INTRODUCTION

Ultrasonic measurements of liquid and liquid mixtures are important to understanding the nature of molecular interactions, industries and chemical applications [1-2]. The ultrasonic velocity, density and viscosity of the binary and ternary liquid mixtures have been studied by various investigators and they have discussed about the interactions between the constituents atoms or molecules [2-4]. The association aspects propanol and there mixtures of polar and non polar components is particular interest due to the strongly associated liquid. It can be associated with any other group having same or different degree of polar interactions [5-9]. Our research group investigates the molecular interactions between the components in binary and ternary mixtures using various methods [10-16]. Methyl benzoate is used in perfumery also use as a solvent and as a pesticide used to attract insects such as orchid bees. Propanol is formed naturally in small amounts during many fermentation processes also used as a solvent in the pharmaceutical industry mainly for resins and cellulose esters. It is a small chain alcohol with three carbon atoms also used the manufacture of various esters, perfumery and flavors. Therefore in order to understanding the intermolecular interactions between the component molecules thorough an ultrasonic measurements of the binary mixtures (propanol + benzene) and ternary mixtures (propanol + methyl benzoate + benzene) at 303K. In the present paper report the results of binary and ternary mixtures.

MATERIALS AND METHODS

AR grade propanol, methyl benzoate and benzene liquids were used. It is purified by standard procedure with purity >99%. The ultrasonic velocities were measured using a single crystal ultrasonic interferometer (Mittal type, Model F-80) at a fixed frequency of 2 MHz frequency. The temperature of the cell was controlled by circulating water through the liquid cell from thermostatically controlled constant temperature water bath. The densities were

measured by 5 ml specific gravity bottle with an accuracy of ± 0.5%. The viscosities have been measured using Ostwald's viscometer with an accuracy ± 0.5%.

Theory and Calculations:
From the experimentally measured values of ultrasonic velocity (u), density (ρ) and viscosity (η), various acoustic parameters are calculated using the following relations 1 to 10 discussed in this investigation given below.

Adiabatic compressibility has been calculated from the speed of sound (u) and density (ρ) of the medium using the relation as

$$\beta = \frac{1}{u^2\rho} \quad (1)$$

Intermolecular free length (L_f) has been evaluated using the standard relation as:

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

Where K_T is a temperature dependent constant known as Jacobson's constant.

The relation for free volume in terms of ultrasonic velocity (U) and viscosity (ρ) of the liquid as:

$$V_f = \left(\frac{M_{eff}U}{\eta K}\right)^{3/2} \quad (3)$$

Here M_{eff} is the effective molecular weight $M_{eff} = \sum m_i x_i$, where m_i and x_i are the molecular weight and mole fraction of the individual components . K is a temperature independent constant which is equal to 4.28×10^9 for all liquids.

Relaxation time can be calculated using viscosity and adiabatic compressibility as:

$$\tau = \frac{3\eta\beta}{4} \quad (4)$$

Where η and β are the viscosity and relaxation time respectively.

The acoustic impedance is the parameter related to elastic properties of the medium and calculated by using the expression

$$Z = u\rho \quad (5)$$

Where ρ - the density and u - the ultrasonic velocity of the solutions.

The Lennard - Jones potential is given by

$$LJP = \frac{6v_m}{V_a} \quad (6)$$

Where, V_m and V_a represent the molar volume and available volume of the mixtures.

Rao noticed that the ratio of temperature coefficient of sound velocity to the expansion coefficient is virtually same for all unassociated organic liquids. According to the Rao

$$R = u^{1/3} V \quad (7)$$

From the sound velocity in liquids, another constant has been suggested by Wada. According to Wada

$$w=\frac{m_{eff}}{\rho}\beta^{-1/7} \quad (8)$$

RESULTS AND DISCUSSION

Ultrasonic velocity (u), density (ρ) and viscosity (η) for the binary mixtures of propanol with benzene, ternary mixtures of propanol with methyl benzoate in benzene at 301 K are shown in table 1. The acoustical parameters were finding from the equation 1 to 10, the data were presented in the table 2 also plotted acoustical parameter with mole fraction are shown in figures 1 to 10.

Table-1 The variation of ultrasonic velocity (u m/s), density (ρ gm/cm^3) and viscosity (η x10^{-3} Nsm^{-2}) of the mole fractions (X_2) of phenol at 301K

X_2	Propanol+Benzene			Propanol+ Methyl benzoate + benzene					
	u_{12}	ρ_{12}	η_{12}	X_1	X_2	X_3	u_{12}	ρ_{12}	η_{12}
0.1	1267	862	0.646	0.05	0.5	0.45	1328	959	0.006
0.2	1258	854	0.737	0.1	0.5	0.4	1317	944	0.012
0.3	1250	845	0.836	0.15	0.5	0.35	1306	929	0.021
0.4	1241	837	0.943	0.2	0.5	0.3	1296	915	0.034
0.5	1232	829	1.06	0.25	0.5	0.25	1285	900	0.051
0.6	1224	821	1.185	0.3	0.5	0.2	1274	886	0.073
0.7	1215	813	1.32	0.35	0.5	0.15	1264	871	0.101
0.8	1207	806	1.465	0.4	0.5	0.1	1253	857	0.135
0.9	1198	798	1.62	0.45	0.5	0.05	1243	843	0.175

The values of adiabatic compressibility (βx10^{-10} kg^{-1}ms^{-2}), free volume (V_f m^3), relaxation time (τ x 10^{14}s), inter molecular free length (L_f X 10^{-11}m), acoustic impedance (Z X10^6 kg m^{-2} sec^{-1}), relative association (R_a), molar volume (V_m m^3), Lennard - Jones Potential (LJP) , Rao constant (R m^3/mole)(m/s)$^{1/3}$, Wadas constant (m^3/mole)(nm^2)$^{1/7}$ find from the relation 1 to 10 given table 2 to 3 for the binary and ternary mixtures.

Table 2 The ultrasonic parameter for the binary and ternary mixtures at 303K

X_1	β	V_f	τ	L_f	Z	V_m	V_a	LJP	R	W
Propanol + Benzene										
0.1	7.23	0.0065	62	5.73	1.09	0.0885	18.42	2.88	0.96	1.79
0.2	7.40	0.0051	73	5.79	1.07	0.0872	18.65	2.81	0.94	1.76
0.3	7.57	0.0040	84	5.86	1.06	0.0860	18.82	2.74	0.93	1.73
0.4	7.76	0.0032	98	5.93	1.04	0.0847	19.01	2.67	0.91	1.7
0.5	7.95	0.0026	112	6.01	1.02	0.0834	19.17	2.61	0.89	1.66
0.6	8.13	0.0021	128	6.07	1.00	0.0820	19.26	2.55	0.88	1.63
0.7	8.33	0.0017	147	6.15	0.99	0.0806	19.39	2.49	0.86	1.6
0.8	8.52	0.0014	166	6.22	0.97	0.0790	19.41	2.44	0.84	1.56
0.9	8.73	0.0011	189	6.29	0.96	0.0776	19.49	2.39	0.82	1.53
Propanol + Methyl benzoate + Benzene										
0.05	5.91	12.88	0.47	5.18	1.274	0.1108	18.8	3.53	1.22	2.31
0.1	6.11	4.44	0.98	5.27	1.243	0.1116	19.7	3.39	1.22	2.31
0.15	6.31	1.87	1.77	5.35	1.213	0.1124	20.7	3.27	1.23	2.32
0.2	6.51	0.89	2.95	5.43	1.186	0.1131	21.5	3.16	1.23	2.32
0.25	6.73	0.47	4.58	5.53	1.157	0.1140	22.4	3.05	1.24	2.33
0.3	6.95	0.27	6.76	5.62	1.129	0.1148	23.4	2.94	1.24	2.34
0.35	7.19	0.16	9.68	5.71	1.101	0.1158	24.3	2.86	1.25	2.34
0.4	7.43	0.10	13.37	5.81	1.074	0.1166	25.3	2.77	1.26	2.35
0.45	7.68	0.07	17.92	5.90	1.048	0.1175	26.2	2.69	1.26	2.36

Ultrasonic velocity is decreases with increasing the mole fractions of propanol, similar trend observed in the density and viscosity values increases. The experimental values are non ideal mixture behavior and this can be attributed to the intermolecular interaction in the propanol with benzene, propanol with benzene in methyl benzoate mixtures. It is based on the pure value of the components. These behaviors indicate the presence of large number molecules in the mixture. The viscosity values increases pointed out the existence of induced dipole – dipole or dipole – dipole

interactions in the systems. Ultrasonic velocity should increase, if the inter molecular free length decreases vice versa. This information was noticed for all the liquid mixtures. In fact, the molecular association between the molecules increases. The ultrasonic velocity decreases, the acoustic impedance, intermolecular free length increases and decrease in adiabatic compressibility is suggested that the component molecules are held close to each other. These shows the strong molecular interaction between the unlike molecules through dipole – dipole interactions. Benzene as non polar liquids the parameters are almost same. This fact is reflected clearly from the values of ultrasonic velocity, intermolecular free length, adiabatic compressibility and acoustic impedance for the binary and ternary liquid mixtures.

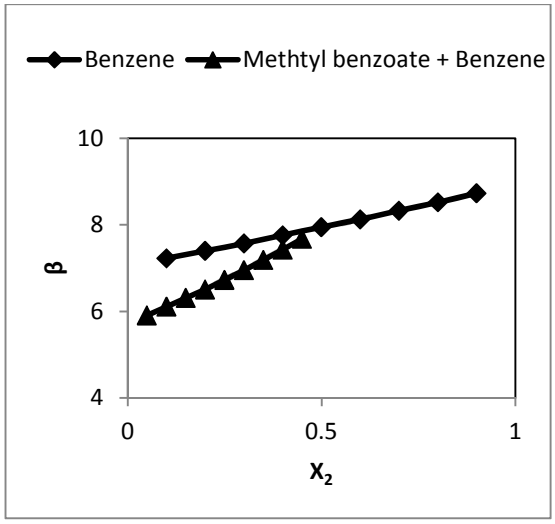

Figure 1 Plots of β versus X_2

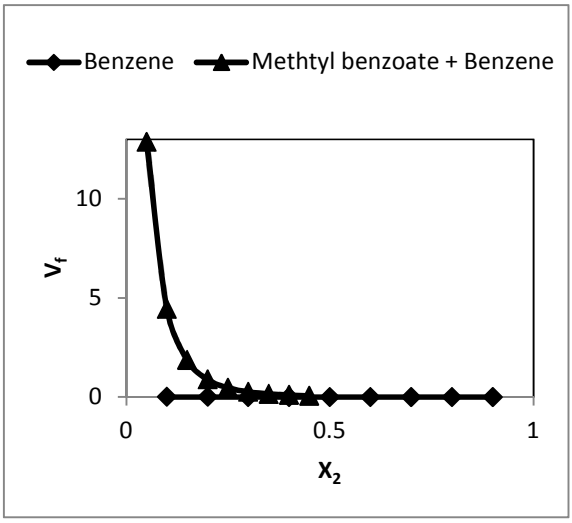

Figure 2 Plots of V_f versus X_2

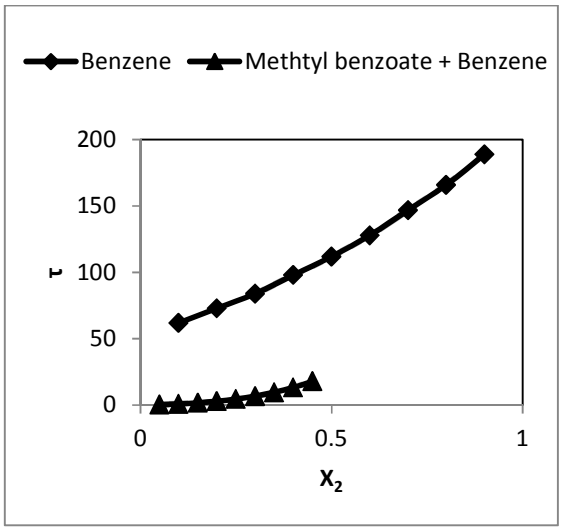

Figure 3 Plots of τ versus X_2

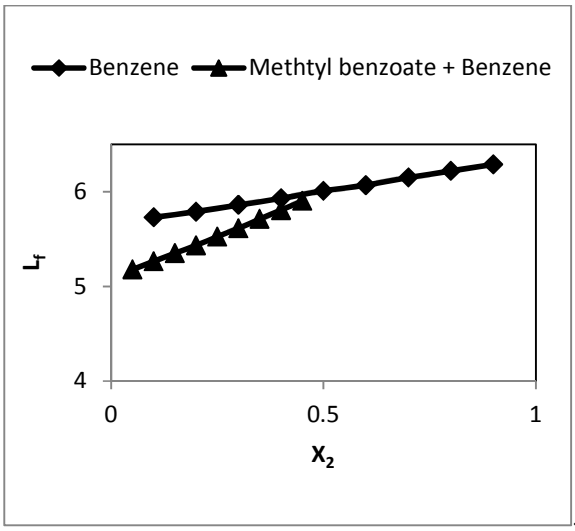

Figure 4 Plots of L_f versus X_2

Propanol generally can be present in polymeric form. In the presence of non polar molecules, they increase molecular interaction due to bond broken. The propanol concentration increases intermolecular hydrogen bonding decreases. The variation acoustic parameter is small indicating the interaction is weaker ultimately ultrasonic velocities of both the components are nearly equal. In this fact is reflected in decrease of ultrasonic velocity and hence increase in inter molecular free length also increase adiabatic compressibility with increasing concentrations of propanol. Acoustic impedance of a material is the resistance exerted by the medium to dislocation of the medium molecules by the sound energy. It is important to measure the acoustic impedance because these studies have shown

that in solvent mixtures when the molecular interaction is occurs; acoustic impedance exhibits a non-linear variation with increasing mole fraction of propanol. This was used as a necessary tool to predict molecular interactions in binary and ternary liquid mixtures. In systems of binary liquid mixtures is always much greater than either of the polar solutes in the inert solvent. Further, the increase in free volume with rise in concentration of propanol in the binary and ternary systems under study, obviously designate the decreasing of magnitude of interactions. The ultrasonic velocity decreases with increase in mole fraction of propanol this suggests that there's different types of molecular interactions between the components. The ultrasonic velocities values vary linearly in these systems behave ideality. These indicate weak interaction occurs in these systems.

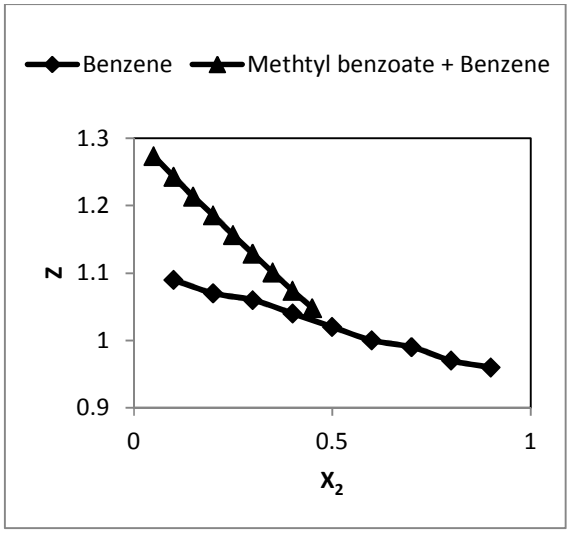

Figure 5 Plots of Z versus X_2

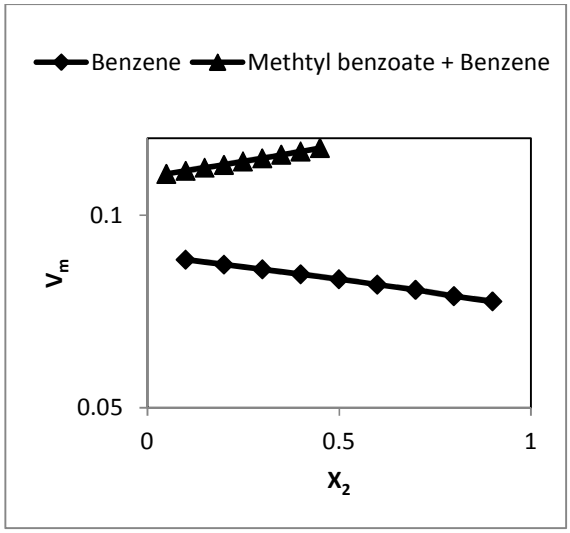

Figure 6 Plots of V_m versus X_2

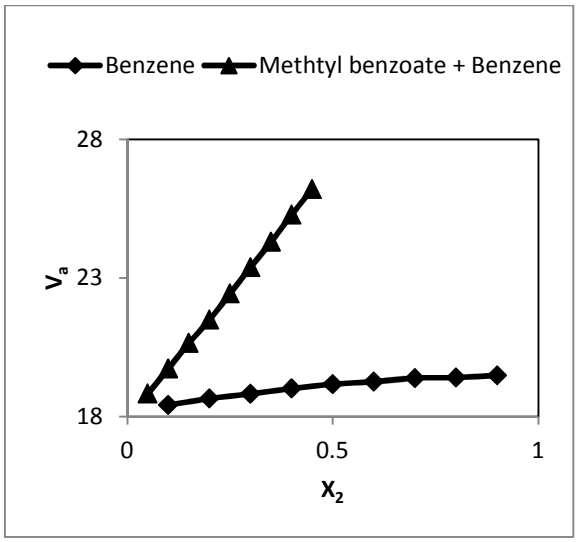

Figure 7 Plots of V_a versus X_2

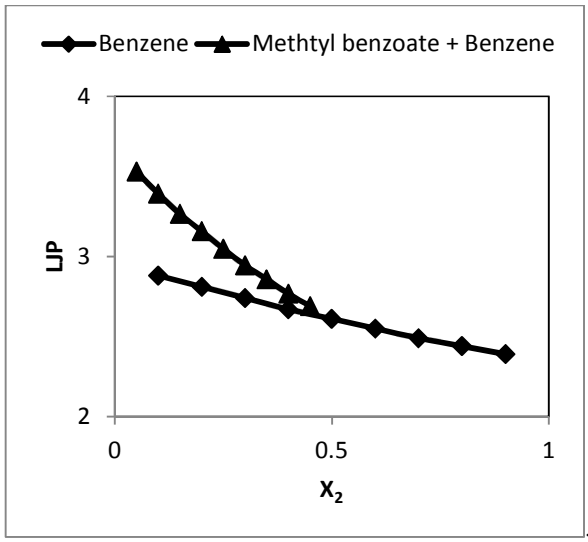

Figure 8 Plots of LJP versus X_2

The adiabatic compressibility values increases for various mole fractions of binary mixtures have been computed from the measured values of ultrasonic velocity and densities. The plots of adiabatic compressibility with mole fraction of the phenol are given in figure 1. In all the systems the value of adiabatic compressibility decreases with increasing concentration of propanol over a range of concentration. This indicates weak interactions exist in these systems. A competition of the value of β in these mixtures suggests that there are compressibility are in the order benzene > benzene + methyl benzoate. The variations in the adiabatic compressibility values in these systems

behave almost ideality. This indicate weak induced dipole-induced dipole exist in these systems. Free volume decreases with increase in concentration and the calculated available volume decreases with increase in concentration of propanol for binary and ternary mixtures as shown in figure 2.

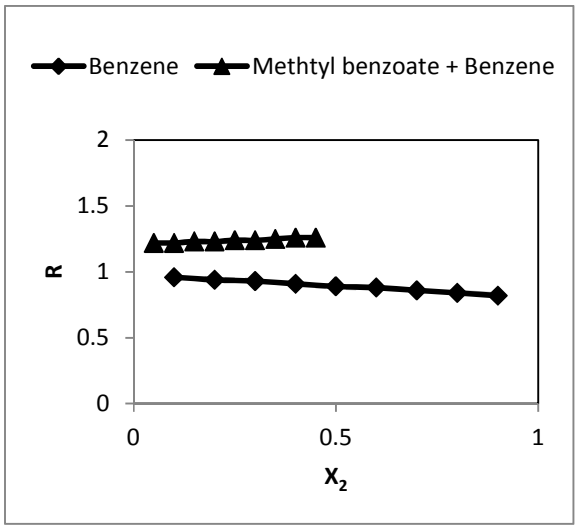

Figure 9 Plots of R versus X_2

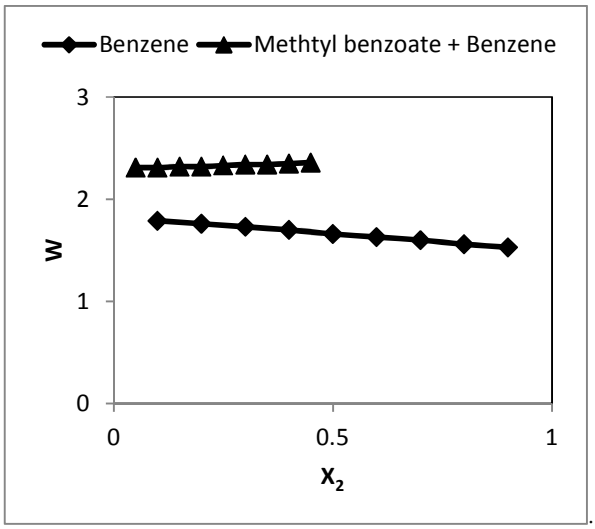

Figure 10 Plots of W versus X_2

The values of relaxation time are given in table 2 and plots shown in figure 3. There are only slight variations in relaxation time values systems. This indicates relatively a weaker interaction exists between the molecules of the two components and stronger intermolecular interactions exist between the molecules of each component. The free lengths of systems is a measure of inter molecular interaction between the liquids. The decrease in free length indicates the weakening of intermolecular interaction. It is given in tables 2 and plots given in figure 4, it is seen that the free length values increase with increase in concentration of propanol. This shows that the intermolecular attraction weakens at higher concentration. The acoustic impedance and adiabatic compressibility show that they exhibit opposite behavior and the behavior is observed in all the liquid mixtures studied (Figure 1and Figure 5). Out of these systems none exhibited a maximum in velocity curve and dip in compressibility curve. This indicates the absence of complex formation. The absence of complex formation is also confirmed by the linear variation of specific acoustic impedance. It is clear from figure 5 that specific acoustic impedance is linear and hence no indication of complex formation. The relative association values in a system can be used to determine the variation in intermolecular interaction and also to establish the existence of similar types of molecular interaction in different mixtures. In the binary and ternary systems studied, the relative association values increase with increase in the mole fraction of the propanol – benzene, propanol + benzene + methyl benzoate systems given in table 2 also shown in figure 6 also find the available volume Vm is plotted in figure 7. The available volume increases with increasing concentration of hexanol. These values increase from unity. This trend suggests that induced dipole –dipole types of molecular interaction exist in all these systems. The LJP values shown in table 2 and the figure 8 indicate that dipole-dipole attractions are stronger than induced dipole-induced dipole attractions. The Rao's constant and Wada's constant are plotted against the concentration of propanol for the binary and ternary systems are shown in given in figure 9 and figure 10. It is clear that the Rao's constant and Wadas constant, the variations of these constants with mole fractions is linear. It was reported that in a binary and ternary liquid mixtures, a linear variations of Rao's constant and Wada's constant with mole fraction shows weak induced dipole-induced dipole interaction in all binary and ternary systems.

CONCLUSION

The ultrasonic velocity, density and viscosity for the mixtures of propanol with benzene, propanol with methyl benzoate in benzene have been made. The acoustical parameters have been calculated from these values. The type of interactions occurs in the binary and ternary liquid mixtures have been explained. It is found that the interaction between unlike molecules increases with the increasing concentration of propanol.

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