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Der Pharmacia Sinica, 2016, 7(1): 1-5

Der Pharmacia Sinica
ISSN: 0976-8688
CODEN (USA): PSHIBD

Molecular interaction studies of methyl acetate with o/p/m-xylene by the ultrasonic measurements

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ABSTRACT

The ultrasonic velocity, density and viscosity are measured for the binary mixtures of methyl acetate with xylene (o, p, and m) were made at 301K. From these measurements the adiabatic compressibility, acoustic impedance, free length, free volume, Wada's constant and Rao constant have been evaluated. The experimental and related acoustical parameters have been utilized to discuss about the molecular interactions. These indicate weak interactions occurred in the systems.

Keywords: Ultrasonic velocity, density, viscosity, Wada's constant, Rao constant

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INTRODUCTION

Ultrasonic measurements of liquids and liquid mixtures are very important due to the molecular interaction between same or different kinds of molecules. The intermolecular interaction in the liquid mixture shows the variation of the physical and chemical properties of the liquid mixtures [1-3]. A liquid mixture consisting of polar-polar and polar - non polar liquids is important in chemical, pharmaceutical applications. The thermodynamic properties of liquid mixtures have been extensively used to understand the molecular interactions due to deviation from ideal liquid mixture behavior [4-6]. Methyl acetate is an important solvent used in paint and nail polish removers etc. The xylene isomer is used as solvent, due to the extensive application of this material it has been used for the present investigation, although several [8-10] investigation were carried out by ultrasonic measurements. This paper reports a systematic investigation of molecular interaction of methyl acetate with xylene isomer through ultrasonic measurements.

MATERIALS AND METHODS

The AR grade samples purchased from the SD fine chemicals Ltd., India. The methyl acetate, o-xylene, p-xylene and m-xylene samples were used. The samples are purified by standard methods and drying before use. The various compositions were prepared by weighing in chemical balance with accuracy 0.0001 gm. The ultrasonic velocity were measured using an ultrasonic interferometer (M-82, Mittal Enterprises), New Delhi) operating at 3MHz with an accuracy of ±1 ms^{-1}. The densities were measured using 25 ml specific gravity bottle and Viscosity has been measured using Ostwald's viscometer. The specific gravity bottle and viscometer were calibrated using purified water. The temperature for all measurements maintained at 301K by circulating water using high precision thermostat also check the purity of the samples by the measurement of density. The purity of the sample is 99.99%.

THEORY AND CALCULATIONS

The following acoustical parameters have been evaluated from the ultrasonic velocity, density and viscosity measurements.

Adiabatic compressibility (β) may even be calculated from the speed of sound and the density of the medium using the equation of Newton and Laplace as

$$\beta = \frac{1}{U^2 \rho} \quad \text{.... (1)}$$

Free volume in terms of ultrasonic velocity (u) and the viscosity of the liquid (η) as

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

Determination of intermolecular free length in liquids and in liquid mixtures has been a subject of considerable interest using semi-empirical relation to accomplish the idea of intermolecular free length in order to report the ultrasonic velocity in liquids.

i.e. $L_f = K_T \sqrt{\beta}$.

.... (3)

The acoustic impedance is the product of the velocity of ultrasound in a medium and density. It can be calculated by the relation.

$$Z = U\rho \quad \text{.... (4)}$$

Relative association can be calculated from the relation

$$R_a = \left(\frac{\rho}{\rho_o} \right) \left(\frac{u_o}{u} \right)^{1/3} \quad \text{.... (5)}$$

ρ and ρ_0 are the densities of the pure liquid and liquid mixture. u and u_o are the ultrasonic velocity of pure liquid and liquid mixtures.

The available volume is a direct measure of compactness and the strength of attraction between the molecules of a liquid and liquid mixture. It can be calculated from Schaafâ's relation

$$V_a = V \left[1 - \left(\frac{u}{u_\infty} \right) \right] \quad \text{.... (6)}$$

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

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

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

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

The adiabatic compressibility , free volume , relaxation time , inter molecular free length , acoustic impedance , relative association , molar volume , Rao constant and Wads constant evaluated from the relation 1- 8 and these values are reported in table 2.

RESULTS AND DISCUSSION

The density, viscosity and ultrasonic velocity values of the binary mixtures of methyl acetate with o, p, m-xylene have been given in table 1 and the various acoustical parameter like adiabatic compressibility, free volume, inter molecular free length, acoustic impedance, relative association, Rao constant and Wada's constant evaluated from the equation 1 to 7 is given in table 2 and plotted in figure 1 to 8.with the mole fraction is shown in the figure 1-5.

Ultrasonic velocity is increases with mole fraction and also there is increase in density and viscosity shown in the table 1 due to the presence of large number of molecules in the methyl acetate - xylene mixture. The increase in viscosity shows the presence of strong interaction between the molecules.

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 methyl acetate with hydrocarbons at 301K

X_2	o-xylene			m-xylene			p-xylene		
	U	ρ	η	u	ρ	η	u	ρ	η
0.1	1318	889	0.097	1329	872	0.111	1321	891	0.101
0.2	1305	894	0.136	1315	879	0.148	1307	896	0.139
0.3	1290	900	0.176	1300	886	0.187	1292	901	0.179
0.4	1275	905	0.214	1284	893	0.224	1277	906	0.217
0.5	1259	910	0.254	1267	900	0.261	1260	911	0.256
0.6	1241	915	0.293	1248	907	0.299	1242	915	0.295
0.7	1220	920	0.336	1225	915	0.341	1221	921	0.337
0.8	1199	925	0.376	1203	922	0.378	1200	926	0.376
0.9	1179	930	0.411	1181	928	0.413	1179	930	0.412

Table 2 Variation of adiabatic compressibility (β 10^{10} kg^{-1}ms^{-2}), free volume (V_f 10^{3}m^3), inter molecular free length (L_f 10^{-10}m), acoustic impedance (Z 10^6 kg m^{-2} sec^{-1}), relative association (R_a), molar volume (V_m m^3), Rao constant (R m^3/mole)(m/s)$^{1/3}$, Wadas constant (m^3/mole)(nm^2)$^{1/7}$ with the mole fractions of methyl acetate with o/p/m-xylene systems

X_2	β	V_f	L_f	Z	RA	V_a	R	W
o-xylene								
0.1	6.39	444.86	5.25	1.18	0.99	19.96	1155	137
0.2	6.48	188.99	5.28	1.17	0.99	20.57	1138	136
0.3	6.57	110.21	5.32	1.17	1	21.15	1121	134
0.4	6.68	72.28	5.36	1.16	1.01	21.82	1103	133
0.5	6.8	52.03	5.41	1.15	1.02	22.48	1086	132
0.6	6.93	38.77	5.46	1.15	1.03	23.17	1068	130
0.7	7.1	30.07	5.53	1.14	1.04	23.96	1050	129
0.8	7.3	23.42	5.61	1.12	1.06	24.92	1031	128
0.9	7.52	18.92	5.69	1.11	1.07	25.83	1013	127
p-xylene								
0.1	6.49	159.05	5.29	1.16	0.97	20.39	1154	137
0.2	6.58	99.93	5.32	1.16	0.98	21.03	1137	136
0.3	6.68	67.96	5.36	1.15	1	21.7	1119	135
0.4	6.79	49.99	5.41	1.15	1.01	22.41	1102	133
0.5	6.92	38.26	5.46	1.14	1.02	23.16	1084	132
0.6	7.08	29.96	5.52	1.13	1.03	24	1065	131
0.7	7.28	23.48	5.6	1.12	1.05	25.03	1046	130
0.8	7.49	19.22	5.68	1.11	1.06	25.98	1027	129
0.9	7.73	16.06	5.77	1.1	1.08	26.9	1008	128
m-xylene								
0.1	6.43	181.6	5.26	1.18	1	20.54	1152	137
0.2	6.53	108.79	5.3	1.17	1	21.21	1134	136
0.3	6.65	71.9	5.35	1.16	1.01	21.91	1117	134
0.4	6.77	52	5.4	1.16	1.02	22.58	1100	133
0.5	6.91	39.07	5.45	1.15	1.03	23.36	1082	132
0.6	7.08	30.35	5.52	1.14	1.04	24.19	1063	131
0.7	7.28	23.79	5.6	1.12	1.06	25.13	1045	130
0.8	7.5	19.3	5.68	1.11	1.07	26.06	1026	129
0.9	7.74	16.08	5.77	1.1	1.08	26.97	1007	128

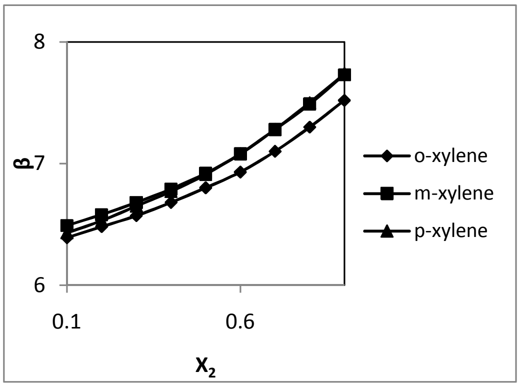

Figure 1 plots of β with X_2

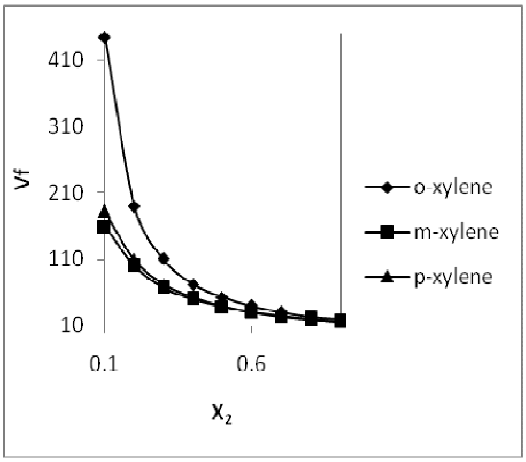

Figure 2 plots V_f Vs X_2

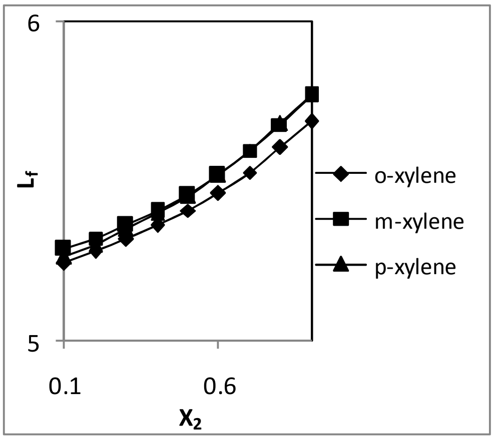

Figure 3 plots of L_f Vs X_2

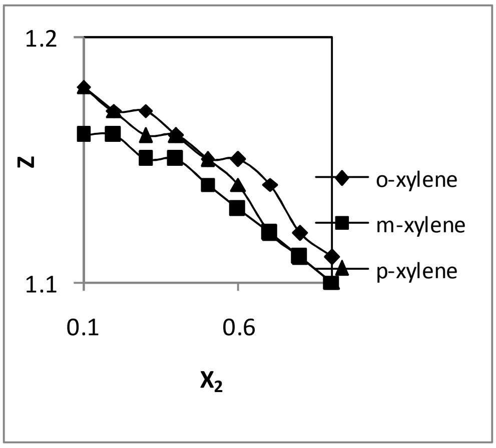

Figure 4 plots of Z with X_2

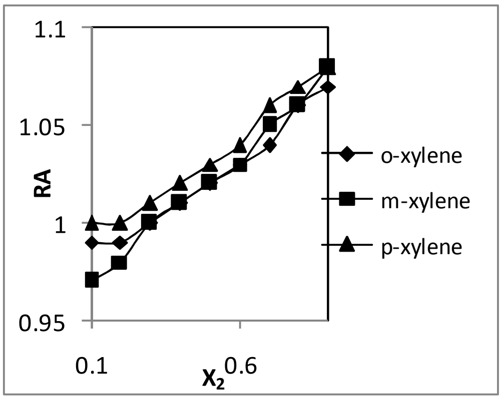

Figure 5 plots of RA with X2

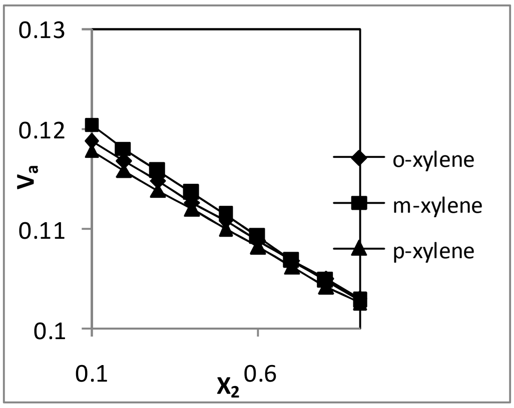

Figure 6 plots of Va with X2

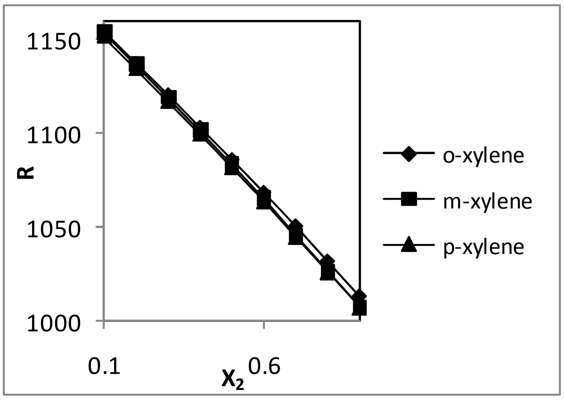

Figure 7 plots of R Vs X_2

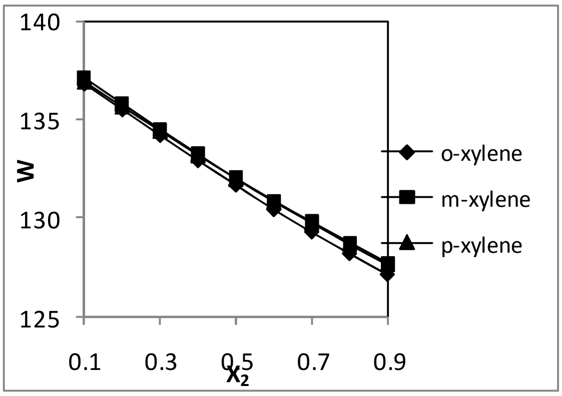

Figure 8 plots of W Vs X2

The adiabatic compressibility decreases with increase in mole fraction of methyl acetate shown in figure 1, which is due to weak molecular interaction between solute and solvent. The free volume decrease with increasing concentration of methyl acetate as given in figure 2, these indicate weak solute – solvent interaction exist in these systems. From the figure 3, it represent the variation of inter molecular free length which is decreases with mole fraction it gives an idea about the molecules with close packing. These indicate that the intermolecular interaction weakens at higher concentration. Linear variation in acoustic impedance indicates the absence of complex formation in the binary mixtures as shown in the figure 4. From the figure 5, the relative association increases with increasing concentration of methyl acetate. The relative association values increase from the unity. These trends suggest weak induced dipole – induced dipole type of molecular interaction occurring in these binary mixtures. Available volume is a measure of density and force of the bonding between molecules of binary mixtures. The available volume decrease with increasing concentration of methyl acetate as given in figure 6, also this indicates that weak solute – solvent interaction exist in these systems The linear variation of Rao and Wada's constant are shown in figure 7 and figure 8. These confirm the weak interaction takes place in all binary mixtures of methyl acetate and o/p/m-xylene mixtures.

CONCLUSION

Densities, viscosities, and ultrasonic velocities for three binary mixtures have been measured. The acoustical parameter like adiabatic compressibility, free volume, intermolecular free length, acoustic impedance, relative association, free volume, Wada's constant and Rao constant for the binary mixtures of methyl acetate with hydro carbon (o, p, m- xylene) were obtained from the experimental results. It has been concluded that induced dipole – dipole interactions occurring in methyl acetate hydro carbon mixtures.

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