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Study of Molecular Interactions in Para Azoxy Anisole (PAA) In Different Solutions

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Abstract:- This paper dwells on the results of the experimental study of three binary mixture i.e., Para-azoxy anisole (PAA)-Benzene (C_6H_6), Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4), Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at 303K, 303K and 304K respectively. The ultrasonic velocity (u) and density (ρ) have been measured in different mole fraction. From these values the acoustical parameters like adiabatic compressibility (β), acoustic impedance (Z) and free length (L_f) have been calculated. And also access Wada's constant (W) and Rao's constant(R). The extent of interactions existing between component molecules has been found.

Keywords:- Binary mixture, Free length of interaction, Wada's constant, Rao's constant, Adiabatic compressibility, Acoustic impedance

I. INTRODUCTION

In recent years, ultrasonic measurements technique has been found to be more powerful and comprehensive tool to detect and assess molecular interactions in binary mixture [1-10], because mixed solvents find practical applications in many industrial and chemical processes. For which ultrasonic velocity measurements are generally carried out at room temperature. The acoustical parameters like adiabatic compressibility (β), acoustic impedance (Z), free length (L_f), Wada's constant (W) and Rao's constant (R) provide the interactions existing between component molecules.

The investigation is carried out to study molecular interactions in the binary liquid mixture of Para-azoxy anisole (PAA)-Benzene (C_6H_6), Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4), Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at the temperature 303K, 303K and 304K respectively.

II. MATERIALS AND METHODS

The ultrasonic velocity of Para-azoxy anisole (PAA) liquid crystal in solutions in high purity Benzene (C_6H_6), Carbon tetrachloride (CCl_4) and 1-4 Dioxane ($C_4H_8O_2$) has been measured at various concentrations and room temperature using interferometer technique at 2 MHz. The ultrasonic velocity is measured with an uncertainty of ±0.3% using single crystal ultrasonic interferometer operating at 2 MHz (Mittal Enterprises, New Delhi) (Model F81). The interferometer calibrated with water and benzene.

Binary mixture are prepared by mixing the liquid crystal and solvent in the standard flasks with airtight caps and mass measured by digital balance with an accuracy of ±1 mg. The uncertainty in the measurement of density and viscosity is of the order of ±0.01 and ±0.001 respectively. The accuracy of measurement in mole fraction is ±0.0001.

In order to calculated the ultrasonic velocity, the total distance d moved by the reflector of the interferometer cell is given by

$d = n\lambda/2$ --(1)

Where λ is wavelength of ultrasonic wave. Because the frequency of the interferometer crystal is accurately known 2 MHz and using λ from Eq. (1), the ultrasonic velocity (u in m/sec) is calculated by the relation

$u = n\lambda$ --(2)

Using the measured values of velocity (u), density (ρ) and viscosity (η) the acoustical parameters can be calculated through the following relations [12,13]

Adiabatic compressibility;

$\beta = 1/u^2\rho$ --(3)

Acoustic impedance;

$Z = u\rho$ --(4)

Free length;

$L_f = K\beta^{1/2}$ --(5)
Where K is temperature dependent constant [value $(93.875+0.345T)10^{-8}$].
Wada's constant;
$W = \beta^{1/7}.V$ --(6)
Rao's constant;
$R = u^{1/3}.V$ --(7)
Where V is molar volume. [14]

Table-1. Variation of ultrasonic velocity, density, molar volume and adiabatic compressibility of Para-azoxy anisole (PAA)-Benzene (C_6H_6), Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4), Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at 303K, 303K and 304K respectively.

Mole fraction	Ultrasonic velocity (u) m/s	Density (ρ)	Molar Volume (V)	Adiabatic compressibility (β)
PAA+ BENZENE (303K)				
0.00176	1244	0.8319	94.274	7.76762E-07
0.00404	1244	0.8327	94.671	7.76016E-07
0.00577	1244	0.8655	91.447	7.46607E-07
0.00898	1252	0.8711	91.524	7.32358E-07
PAA+ CCL4 (303K)				
0.00059	904	1.3172	116.839	9.28991E-07
0.00284	915	1.533	100.541	7.7914E-07
0.00624	912	1.5743	98.126	7.637E-07
0.01103	910	1.6219	95.561	7.44549E-07
PAA+ C4H8O2 (304K)				
0.00081	1312	1.0242	86.694	5.67215E-07
0.0012	1314	1.0227	86.538	5.66319E-07
0.00178	1316	1.0213	86.596	5.65373E-07
0.0035	1317	1.0238	86.65	5.63136E-07

Table-2. Variation of Acoustic impedance (Z), Free length (L_f), Wada's constant (W) and Rao's constant (R) of Para-azoxy anisole (PAA)-Benzene (C_6H_6), Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4), Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at 303K, 303K and 304K respectively.

Mole fraction	Acoustic impedance (Z)	Free length (L_f)	Wada's Constant (W)	Rao's Constant (R)
PAA+ BENZENE (303K)				
0.00176	0.00103488	1.749E-09	12.635	1013.91
0.00404	0.00103588	1.748E-09	12.6865	1018.18

0.00577	0.00107668	1.714E-09	12.187	983.504
0.00898	0.00109062	1.698E-09	12.1637	986.438
PAA+ CCL4 (303K)				
0.00059	0.00119075	1.912E-09	16.0648	1129.74
0.00284	0.0014027	1.751E-09	13.4808	976.076
0.00624	0.00143576	1.734E-09	13.1195	951.588
0.01103	0.00147593	1.712E-09	12.7302	926.036
PAA+ C4H8O2 (304K)				
0.00081	0.00134375	1.497E-09	11.1088	949.075
0.0012	0.00134383	1.496E-09	11.0863	947.848
0.00178	0.00134403	1.494E-09	11.0911	948.964
0.0035	0.00134834	1.492E-09	11.0917	949.796

Figure 1. Variation of Wada's constant with Mole Fraction (Para-azoxy anisole (PAA)-Benzene (C_6H_6)at303K)

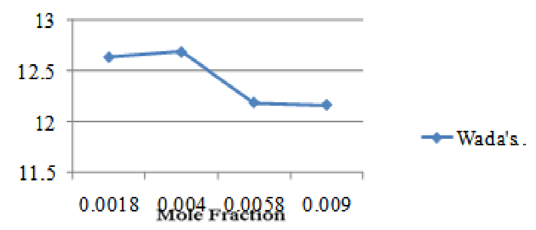


Figure 2. Variation of Wada's constant with Mole Fraction (Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4) at 303K)

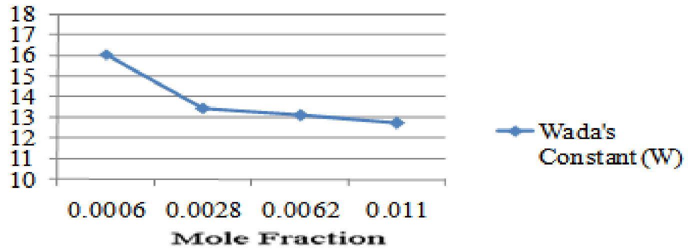


Figure 3. Variation of Wada's constant with Mole Fraction (Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at 304K)

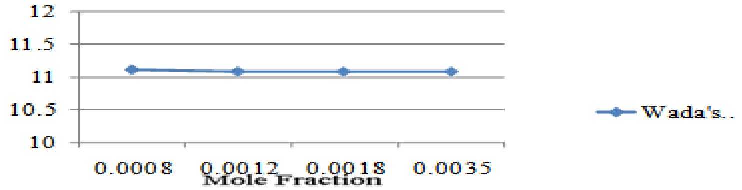


Figure 4. Variation of Rao's constant with Mole Fraction (Para-azoxy anisole (PAA)-Benzene (C_6H_6) at 303K)

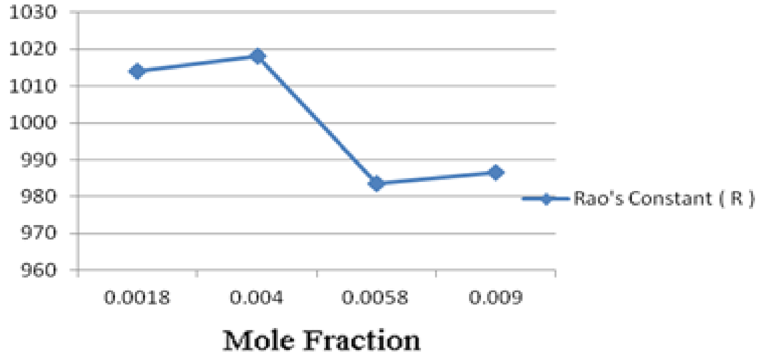


Figure 5. Variation of Rao's constant with Mole Fraction (Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4) at 303K)

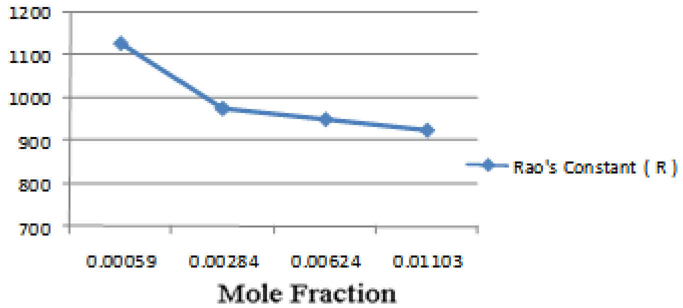
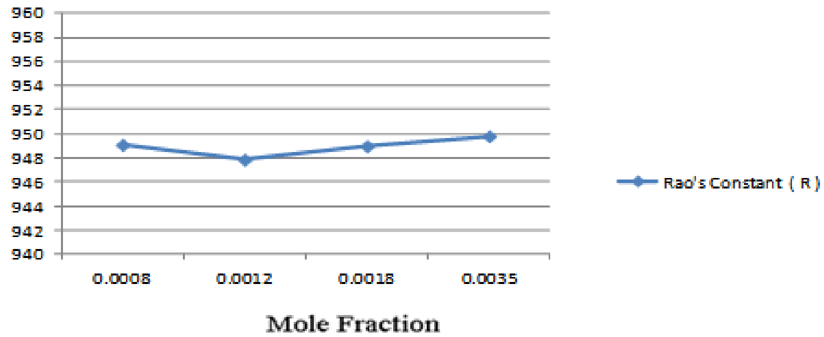


Figure 6. Variation of Rao's constant with Mole Fraction (Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at 304K)



III. RESULT AND DISCUSSION

The experimentally measured values of ultrasonic velocity (u), density (ρ), molar volume and adiabatic compressibility (β) in Table-1 for Para-azoxy anisole (PAA)-Benzene (C_6H_6), Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4), Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) at 303K, 303K and 304K respectively. The calculated values of acoustic impedance (Z), free length (L_f), Wada's constant (W) and Rao's constant (R) in Table-2.

The variation of Wada's constant with mole fraction is shown in Figure-1, 2 and 3 and the variation of Rao's constant with mole fraction is shown in Figure-4, 5 and 6.

As regards sound velocity in Benzene (C_6H_6) increases with density (0.8711), the sound velocity in Carbon tetrachloride (CCl_4) it initially increases and then decrease with increase in density, where as in 1-4 Dioxane ($C_4H_8O_2$) the sound velocity continuously increases with increase in density.

Comparing the three solvents 1-4 Dioxane ($C_4H_8O_2$) is a good solvents that can dissolve Para-azoxy anisole (PAA). In 1-4 Dioxane ($C_4H_8O_2$) mixture the Para-azoxy anisole (PAA) is completely dissolved and so no chance of hydrogen bond ruptures and only the interaction with the Para-azoxy anisole (PAA) and the active group of 1-4 Dioxane ($C_4H_8O_2$), which are mostly dispersive in nature. The increase in mole fraction of Para-azoxy anisole (PAA) increases the net dispersive interactions and hence the velocity continuosly increases as observed. The case of Benzene (C_6H_6) and Carbon tetrachloride (CCl_4) is different due to less salvation tendency.

From Table-1, it is observed that adiabatic compressibility (β) increases with increase in concentration of Benzene (C_6H_6) and decreases with increase in concentration of Carbon tetrachloride (CCl_4) and 1-4 Dioxane ($C_4H_8O_2$).

In Table-2 for Para-azoxy anisole (PAA)-Benzene (C_6H_6), Para-azoxy anisole (PAA)-Carbon tetrachloride (CCl_4 and Para-azoxy anisole (PAA)-1-4 Dioxane ($C_4H_8O_2$) mixtures the acoustic impedance (Z) increases with increase in concentration and free length (L_f), Wada's constant (W) and Rao's constant (R) decrease with increase in concentration.

IV. CONCLUSION

Solute-solvent interactions are dominating over the solute-solute interaction [15] over the whole concentration range. 1-4 Dioxane ($C_4H_8O_2$) is a good solvent for Para-azoxy anisole (PAA). Components maintain their individuality in the mixture. All the experimental determinations of adiabatic compressibility (β), molar volume (V), free length (L_f), acoustic impedance (Z), Wada's constant (W) and Rao's constant (R) are strongly correlated with each other.

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