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Acoustic Studies of Molecular Interaction in 1,1`-Diacetyl Ferocene (DAF) in Different Solutions

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ABSTRACT: *The acoustic studies for three binary mixture namely, 1,1`-Diacetyl ferocene (DAF)-Benzene ($C_6H_6$), 1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) and 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) have been determined at three different temperatures. The measured speed of sound (u), density (ρ) in different mole fraction and the computed acouctical parameters like adiabatic compressibility (β), acoustic impedance (Z) and free length (L_f) have been calculated and also find Wada's constant (W) and Rao's constant (R). The trend in acoustical parameters indicates that there are molecular interactions between the components.*

KEYWORDS: *Acoustic impedance, Adiabatic compressibility, Binary mixture, Free length of interaction, Rao's constant, Wada's constant*.

I. INTRODUCTION

The ultrasonic study of properties of liquid mixtures and solutions find direct application in chemical industry.[1,2] Binary liquid mixture consisting of polar and non polar components are remarkable importance in industries. Transport and thermodynamics properties of liquid mixtures have been extensively used to study the departure a real liquid mixture behavior from ideality.[3-6]Volumetric, viscometric and ultrasonic studies of liquid mixtures have gained much significance in finding the nature of molecular interactions and investigating the physic-chemical accepts of binary liquid systems.[7-10] The ultrasonic technique has been found to be more powerful and comprehensive tool in understanding the solute-solvent interaction.[11]

The extent of molecular interactions has been found in the binary liquid mixtures of 1,1`-Diacetyl ferocene (DAF)-Benzene ($C_6H_6$), 1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) and 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) in the temperatures 295K, 303K and 310K respectively.[12]

II. MATERIALS AND METHODS

All the chemicals used were of Analytical Reagent (AR) grade with minimum assay of 99.9%. The ultrasonic velocity (u) in mixtures have been measured using an ultrasonic interferometer (Mittal type Model F81) working at 2 MHz fixed frequency with an accuracy of ±0.1 m/sec. The density of solution (mixture) was determined using Pycknometer by relative measurement method with an accuracy of ±0.0001 NSm^{-2}.[13]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)

From Eq. (1), wavelength λ can be calculated. Because the frequency of the interferometer crystal is accurately known 2 MHz, the ultrasonic velocity (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 diabatic compressibility (β), acoustic impedance (Z), free length (L_f), Wada's constant (W) and Rao's constant (R) have been calculated using following expressions.

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

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

$L_f = K\beta^{1/2}$ --(5)

$W = \beta^{1/7}.V$ --(6)

$R = u^{1/3}.V$ --(7)

Where K is temperature dependent constant [value $(93.875+0.345T)10^{-8}$] and V is molar volume.

Table 1. Variation of ultrasonic velocity, density, molar volume and adiabatic compressibility of 1,1`-Diacetyl ferocene (DAF)-Benzene ($C_6H_6$), 1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) and 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) in the temperatures 295K, 303K and 310K respectively

Mole fraction	Ultrasonic velocity (u) m/s	Density (ρ)	Molar Volume (V)	Adiabatic compressibility (β)
DAF+ BENZENE (295K)				
0.000078	1310	0.8756	89.454	6.65506E-07
0.000101	1310	0.8756	89.169	6.65506E-07
0.0001185	1302	0.876	89.056	6.73401E-07
0.0001839	1317	0.877	89.254	6.57399E-07
DAF+ CCL4 (303K)				
0.0005484	908	1.5671	97.205	7.73983E-07
0.001888	909	1.5766	97.71	7.67628E-07
0.002743	911	1.5805	97.546	7.62375E-07
0.004698	913	1.5977	96.645	7.50867E-07
DAF+ C4H8O2 (310K)				
0.0003	1300	1.017	86.694	5.81825E-07
0.0006	1309	1.0195	86.538	5.72445E-07
0.00097	1319	1.0196	86.596	5.63742E-07
0.00154	1306	1.0203	86.65	5.74627E-07

Table 2. Variation of Acoustic impedance (Z), Free length (L_f), Wada's constant (W) and Rao's constant (R) of 1,1`-Diacetyl ferocene (DAF)-Benzene ($C_6H_6$), 1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) and 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) in the temperatures 295K, 303K and 310K respectively

Mole fraction	Acoustic impedance	Free length	Wada's Constant (W)	Rao's Constant(R)
DAF+ BENZENE (295K)				
7.8E-05	0.00114704	1.596E-09	11.7272	978.792
0.0001	0.00114704	1.596E-09	11.6898	975.673
0.00012	0.00114055	1.606E-09	11.6947	972.449
0.00018	0.00115501	1.586E-09	11.6805	978.34
DAF+ CCL4 (303K)				
0.00055	0.00142293	1.746E-09	13.0212	941.277
0.00189	0.00143313	1.738E-09	13.0734	946.514
0.00274	0.00143984	1.732E-09	13.0387	945.618
0.0047	0.0014587	1.719E-09	12.8902	937.568
DAF+ C4H8O2 (310K)				
0.0003	0.0013221	1.532E-09	11.1492	946.172
0.0006	0.00133453	1.519E-09	11.1034	946.644
0.00097	0.00134485	1.508E-09	11.0865	949.685
0.00154	0.00133251	1.522E-09	11.1238	947.145

Figure 1. Variation of Wada's constant with Mole Fraction (1,1`-Diacetyl ferocene (DAF)-Benzene (C_6H_6) at 295K)

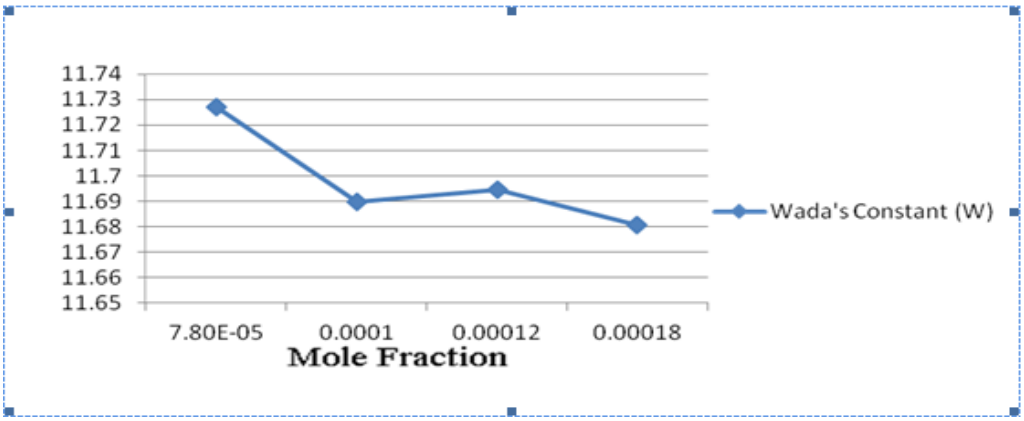


Figure 2. Variation of Wada's constant with Mole Fraction (1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) at 303K)

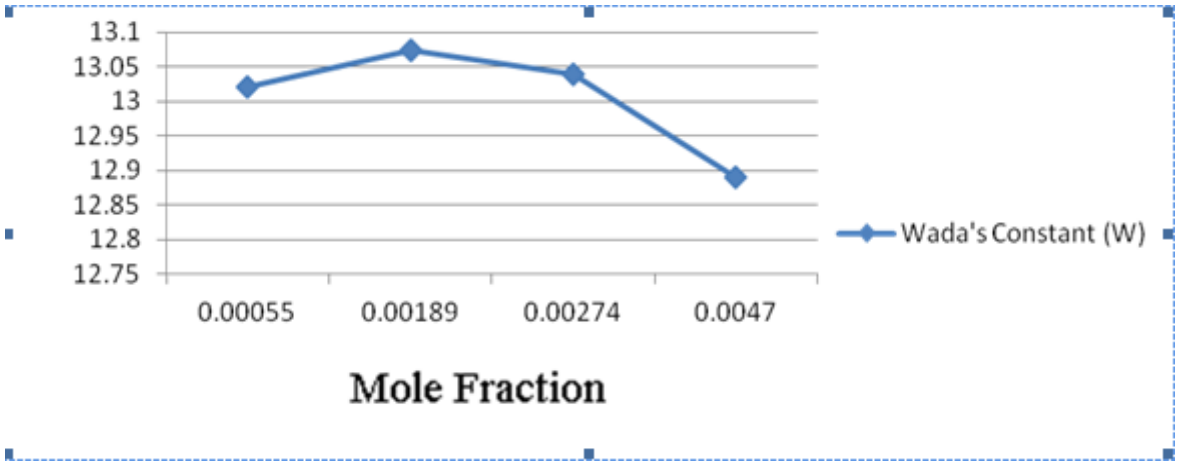


Figure 3. Variation of Wada's constant with Mole Fraction 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) at 310K)

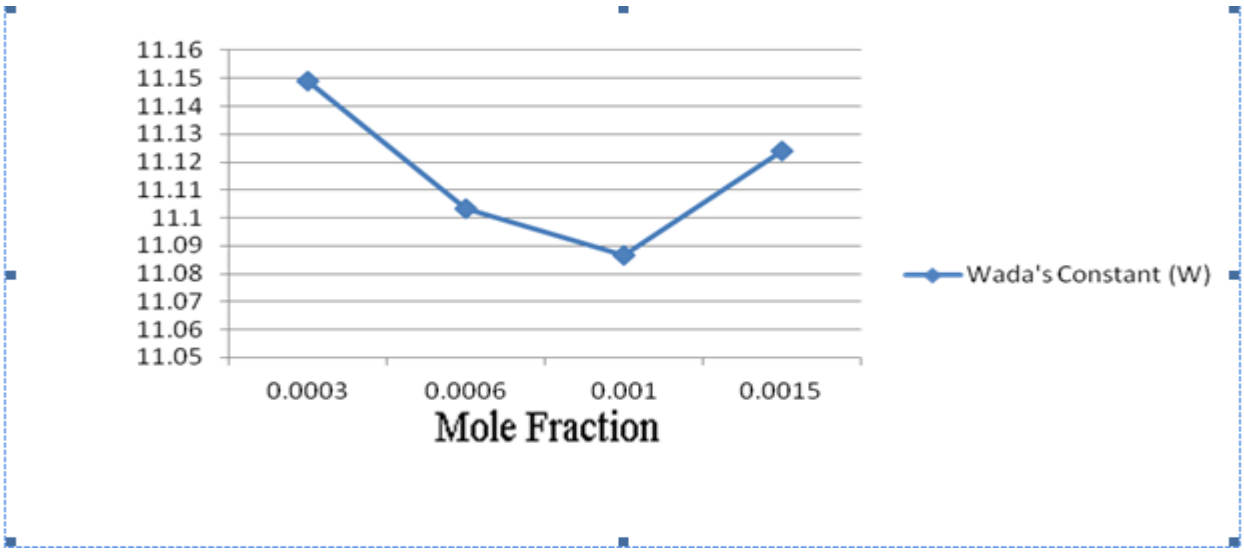


Figure 4. Variation of Rao's constant with Mole Fraction (1,1`-Diacetyl ferocene (DAF)-Benzene (C_6H_6) at 295K)

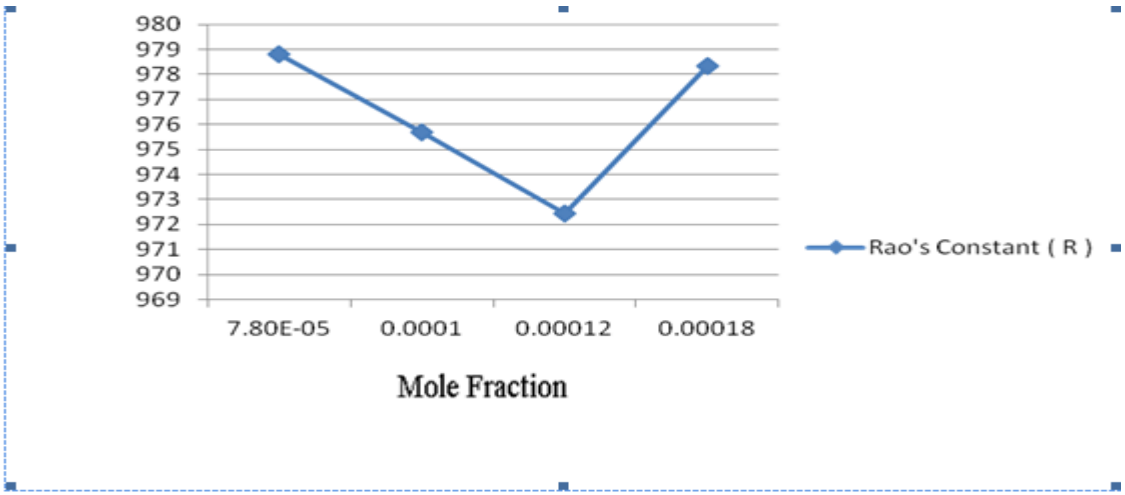


Figure 5. Variation of Rao's constant with Mole Fraction (1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) at 303K)

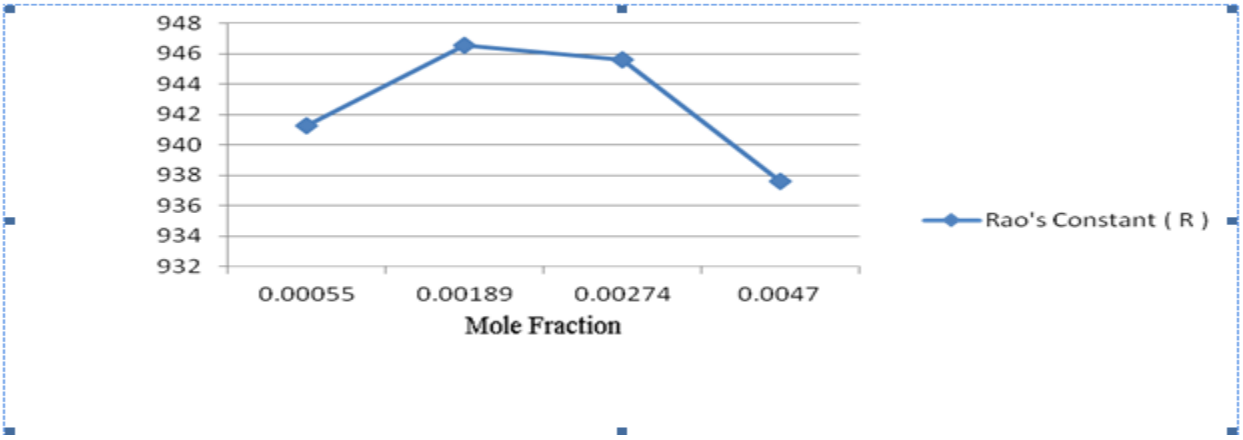
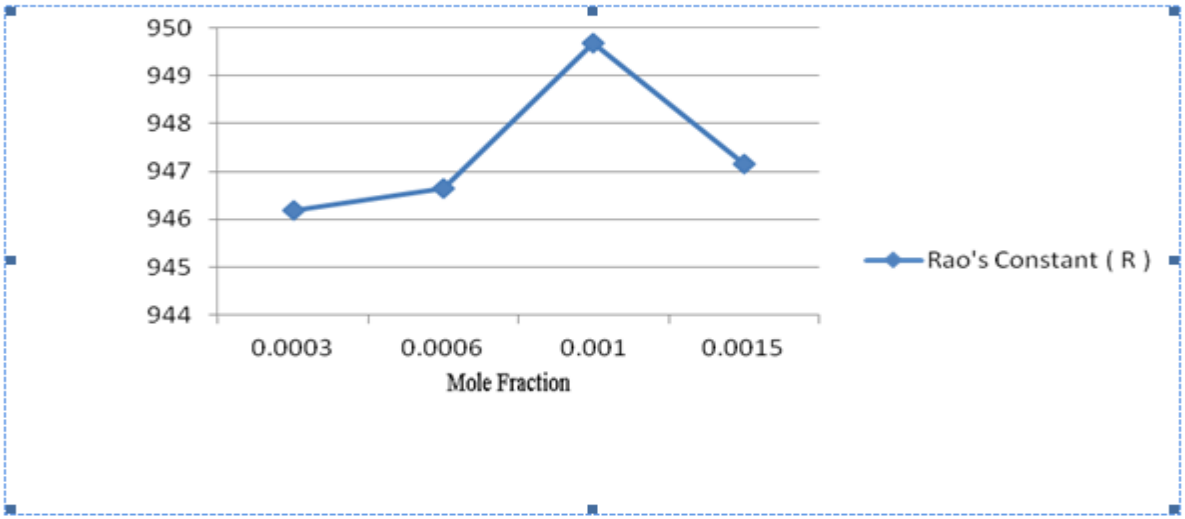


Figure 6. Variation of Rao's constant with Mole Fraction 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) at 310K)



III. RESULT AND DISCUSSION

Table-1 contain the experientially measured values of ultrasonic velocity (u), density (ρ), molar volume (V) and adiabatic compressibility (β). Table-2 contain the calculated values acoustic impedance (Z), free length (L_f), Wada's constant and Rao's constant (R) for 1,1`-Diacetyl ferocene (DAF)-Benzene ($C_6H_6$), 1,1`-Diacetyl ferocene (DAF)-Carbon tetrachloride (CCl_4) and 1,1`-Diacetyl ferocene (DAF)-1-4 Dioxane ($C_4H_8O_2$) in the temperatures 295K, 303K and 310K respectively.Figure-1, 2 and 3 shows the variation of Wada's constant (W) with mole fraction and Figure-4, 5 and 6 shows the variation of Rao's constant with mole fraction.As regards ultrasonic velocity (u) in Benzene (C_6H_6) decrease in density (0.876) and then increases, the ultrasonic velocity in Carbon tetrachloride (CCl_4) continuously increases with increase in density, where as in 1-4 Dioxane ($C_4H_8O_2$) the ultrasonic velocity increases initially and then decreases with increase in density. Comparing the three solvents Carbon tetrachloride (CCl_4) is a good solvents that can dissolve 1,1`-Diacetyl ferocene (DAF). In Carbon tetrachloride ($CCl_4$) mixture the 1,1`-Diacetyl ferocene (DAF) is completely dissolved and so no chance of hydrogen bond rupture and only the interaction with the 1,1`-Diacetyl ferocene (DAF) mostly dispersive in nature. The increases in mole fraction of 1,1`-Diacetyl ferocene (DAF) increase the net dispersive interactions and hence the velocity continuously increases as observed. In case of Benzene (C_6H_6) and 1-4 Dioxane ($C_4H_8O_2$) is different due to less salvation tendency.

IV. CONCLUSION

Solute-solvent interactions are dominating over the solute-solute interaction [14] is a good solvent for 1,1`-Diacetyl ferocene (DAF) components maintain their individuality in the mixture. 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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