DIELECTRIC STUDY OF LORAZEPAM-METHANOL MIXTURE USING TDR METHOD AT 293K

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Abstract: The dielectric Parameters had been decided for mixture of lorazepam-methanol, with concentration of 0, 20, 40, 60, 80 & 100% withinside the frequency variety of 10MHz to 50GHz at temperature of 293K by time domain reflectometry (TDR). The static permittivity and relaxation time had been used to obtain the excess permittivity, excess inverse relaxation time, Bruggeman factor, Kirkwood factor and thermodynamic parameters. A change in dielectric constant and relaxation time, with volume fraction of methanol confirms structural formation because of intermolecular interaction among methanol and lorazepam. The change in factors for varioust mole fraction of methanol in the binary mixture noticed in the paper.

Keywords: Dielectric, Lorazepam, Methanol, 293K.

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1. INTRODUCTION

Dielectric research were finished substantially to apprehend intermolecular interplay and dynamics of the liquid mixture [1-4] using time domain reflectometry. The present study reveals molecular interaction between same functional group [-OH] of the normal alcohol with different molecular size (carbon chain), on the basis of evaluation of static permittivity, relaxation time, Bruggeman factor and thermodynamic parameters [5].

EXPERIMENTAL MATERIAL

The chemical utilized for this work are lorazepam and methanol, are of spectroscopic grade, obtained commercially with 99% purity and used without further purification. The solutions were prepared at six different compositions in steps of 20 % by volume. Lorazepam ($C_{15}H_{10}Cl_2N_2O_2$), is a medicine offered below the brand name. It is used to deal with tension disorders, hassle sleeping It is also used, along with other treatments, for acute coronary syndrome due to cocaine use. It is available as a generic medication [6]. Methanol (CH_3OH) is a colorless, clear liquid. It has repulsive pr alcoholic odor, flammable. Methanol mixes easily with water. It takes place evidently in humans, animals and plants. Many fruits, vegetables, fermented beverages and soda sweetened with aspartame offer a supply of methanol withinside the diet. Methanol is an crucial industrial chemical. It is used as a solvent [7]. Above binary systems are studied for 06 different concentrations (0, 20, 40, 60, 80 and 100%) over the frequency range of 10 MHz to 50 GHz. Temperature dependent variations in dielectric parameters at temperature 293K also reported for the systems.

The volume fractions are converted to mole fractions for further calculations. Using this volume percentage the weight fraction is calculated [8] as

$$X_A = \frac{V_A \rho_A}{[(V_A \rho_A) + (V_B \rho_B)]} \quad (1)$$

where, V_A and V_B are the volume and ρ_A and ρ_B is the density of liquid A(Lorazepam) and B (Methanol) respectively.

APPARATUS

The complex permittivity spectra are studied by using Time Domain Reflectometry. (T.D.R.). The Tektronix Digital Serial Analyzer sampling Oscilloscope (DSA8200) with 80E08 TDR Module has been used. Research work experimental part done at School of physics, Swami Ramanand Teerth Marathwada University. Nanded. Maharashtra. India. It generates a quick repetitive voltage pulse become fed via coaxial line gadget of impedance 50Ω. The time window used for the test is stored at 2 ns. The pondered pulse with out pattern and with pattern are digitized in 2000 factors and transferred to laptop via USB

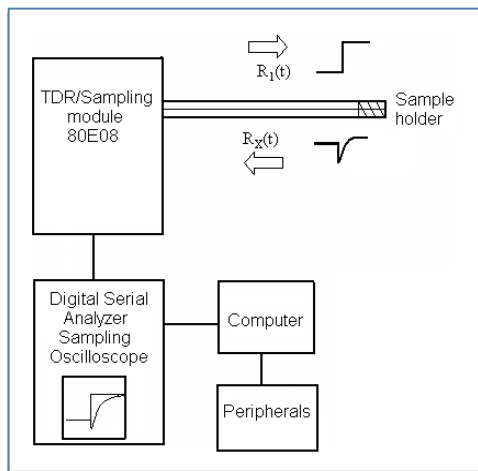device. TDR has up to 30GHz Bandwidth with 20ps reflected rise time and 18ps incident rise time [9].

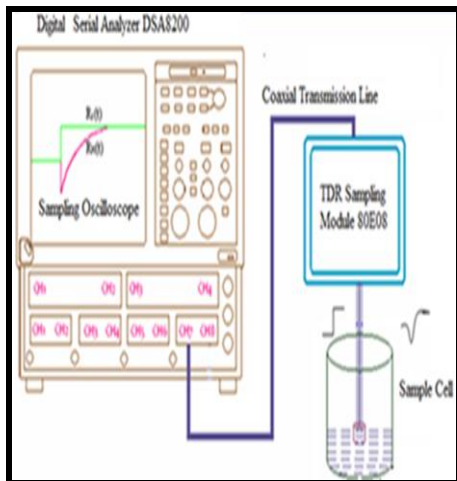**Fig.1** *TDR Experimental block diagram.*

Fig.2 *Experimental setup for TDR*

DATA ANALYSIS

The time based information had been processed to obtain complex reflection coefficient spectra, $\rho^*(\omega)$ over the frequency varies from 10 MHz to 50 GHz use of Fourier transformation [10,11] as

$$\rho^*(\omega) = \left[\frac{c}{j\omega d}\right]\left[\frac{\rho(\omega)}{q(\omega)}\right] \quad (2)$$

Where, $\rho(\omega)$ and $q(\omega)$ are Fourier transforms of $[R_1(t) - R_x(t)]$ and $[R_1(t) + R_x(t)]$, respectively. C represents velocity of light, ω is angular frequency and d indicate effective pin length and j = root (-1). The complex permittivity spectra [12]$\varepsilon^*(\omega)$ obtained from the reflection coefficient spectra $\rho^*(\omega)$ through the use of a bilinear calibration method. The experimental values of $\varepsilon^*(\omega)$ are fitted by Debye equation [13].

$$\varepsilon^*(\omega) = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 + j\omega\tau} \quad (3)$$

where, ε_0, ε_∞ and τ as fitting parameters. The value of ε_∞ was kept to be constant as the fitting parameters are not sensitive to ε_∞. Dielectric parameters are determined by suing non-linear least squares fit method [14].

2. RESULT AND DISCUSSION

Table 1. Static permittivity and Relaxation Time of binary mixture of Lorazepam + Methanol.

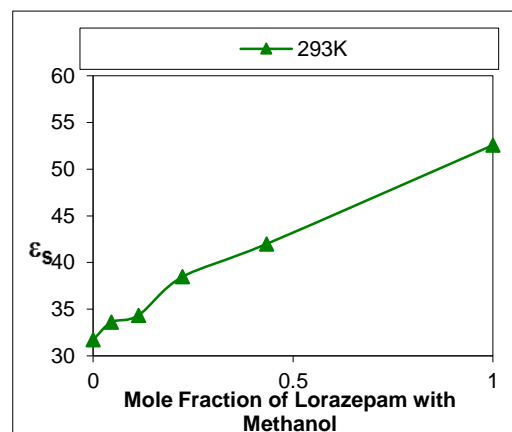| Mole Fraction of Lorazepam	293K	
	ε_s	τ (ps)
0	31.69	49.94
0.046	33.58	53.14
0.113	34.32	55.59
0.223	38.45	57.55
0.434	41.98	58.33
1	52.58	67.13

Figure 3. Change *of static dielectric constant (ε_s) as a characteristic of mole fraction of Lorazepam at temperature 293K.*
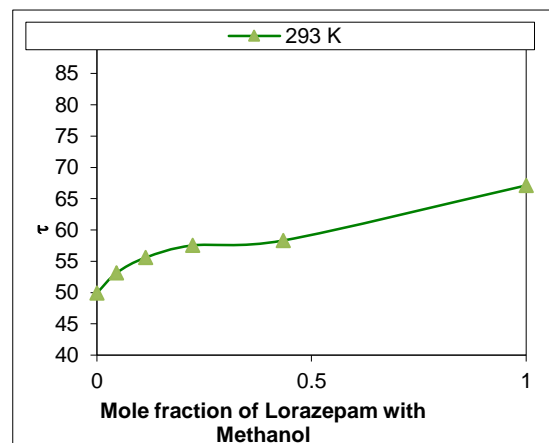

Figure 4. *Change of relaxation time (τ) as a characteristic of mole fraction of Lorazepam at temperature 293K.*

The static dielectric constant (ε_s)and relaxation time (τ) noted by using experimental inputs with the Debye equation are indexed in Table 1 It may observed that there is nearly linear relationship among the values of static dielectric constant (ε_s) with concentration of Lorazepam in the mixtures. As the mole fraction of Lorazwpam increases, the ε_s increases. This indicate that there is well built intermolecular interaction among the molecules of mixture. Likewise relaxation time (τ) increases. This recommend well built intermolecular interaction among Lorazepam and Methanol molecules [15]. The easily rotation of molecules recommended by static permittivity and relaxation time increases with increase in mole fraction and temperature of the system studied. [16].
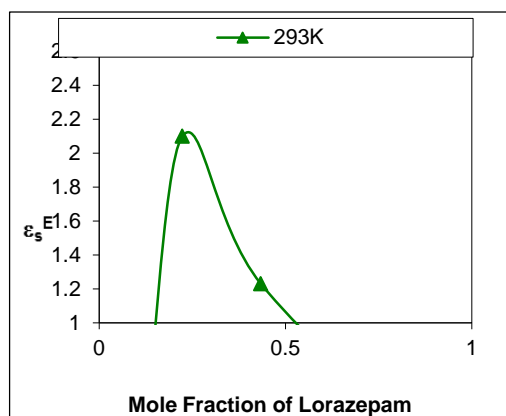
EXCESS PARAMETERS

Figure 5. *Change of excess permittivity (ε_s^E) as a characteristic of mole fraction (x_2) of Lorazepam at temperature 293K.*
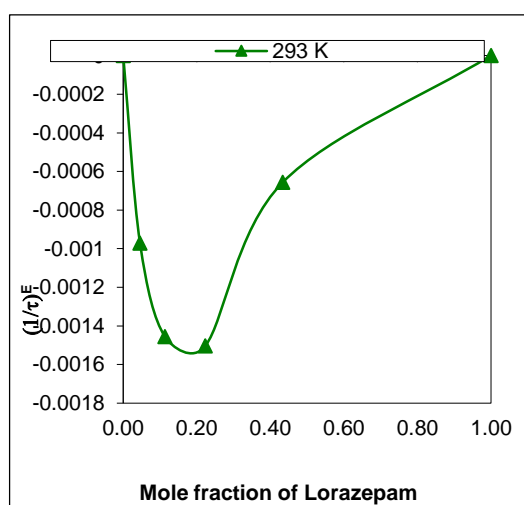

Figure 6. Change *of excess inverse relaxation time $(1/\tau)^E$, as a characteristic of mole fraction (x_2) of Lorazepam at temperature 293K.*

From figure 5 it is observed that for all concentration of Lorazepam $(\varepsilon_s)^E$ is positive in the mixture. This indicates that the molecules of mixture can shape multimeric systems in this kind of manner that there's growth in variety of effective dipoles [17-19]. This is because of the similar alignment (parallel) of the dipoles in the mixture. For all the concentration the curves are more deviated at Methanol rich region.

The behavior in $(1/\tau)^E$ is as shown from figure 6. The dipole rotation in the system is indicated by all negative value of $(1/\tau)^E$ [20].
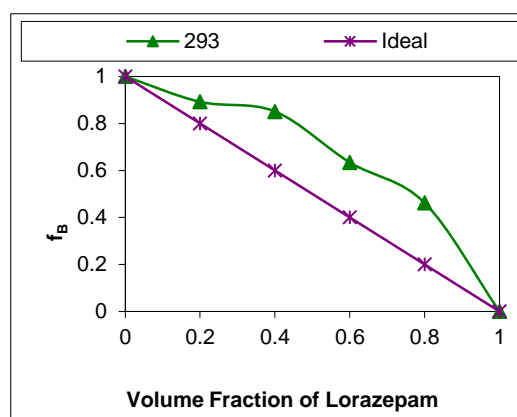
BRUGGEMAN FACTOR

Figure 7. *The Bruggeman plot for binary mixture of lorazepam-methanol.*

From the figure 7 it is observed that, f_B shows a deviation to upper side from the ideal Bruggeman behavior [21]. Indicate effective volume of solvent gets enhanced in the presence of solute. The effective volume value of Bruggeman parameter get less than one. This confirms intermolecular interaction is strong. Furthermore values of (f_B) becomes low with raise in temperature, which shows temperature dependent nature of molecular interactions [22].
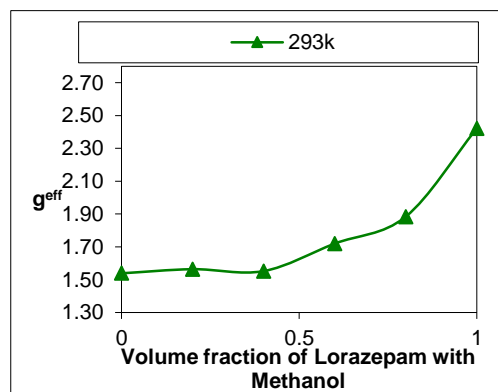
KIRKWOOD CORRELATION FACTOR

Figure 8. *Change of Kirkwood correlation factor 'g^{eff} ' verses volume fraction of Lorazepam in Methanol at temperature 293K.*
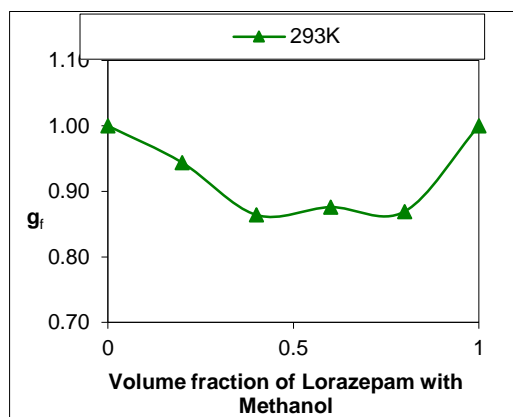

Figure 9. *Change of Kirkwood correlation factor g$_f$ with change in volume characterisitc of Lorazepam in Methanol at temperature 293K.*

The values of g^{eff} are all positive and increases in the range from 1.5 to 2.6 at 293K temperature. The values confirm the bond is form with hydrogen in pure Methanol system. As the values are more than 1, represents effective dipole become larger as compare to pure liquid, and orientation of electric dipole is parallel. [23, 24]. The corresponding values for Lorazepam are indicating weak dipole-dipole interaction resulting formation of antiparallel arrangement of dipoles in the pure system of Lorazepam [25].

The ideal mixture has value of g$_f$ is unity, figure 9 shows change form unity represents , between the two components of mixture the interaction takes place.. The orientation of effective dipole as compare to the pure liquid more, since obsrved g$_f$ value more than one. [26-28].
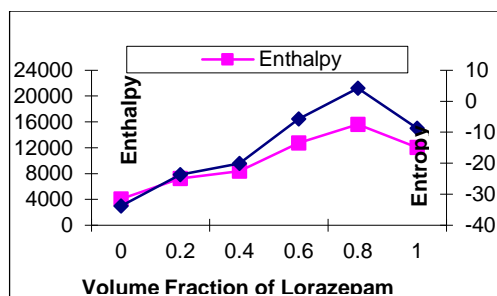
THERMODYNAMIC PARAMETERS

Figure 10. *Enthalpy (ΔH) and Entropy (ΔS) of Lorazepam + Methanol Binary mixture.*
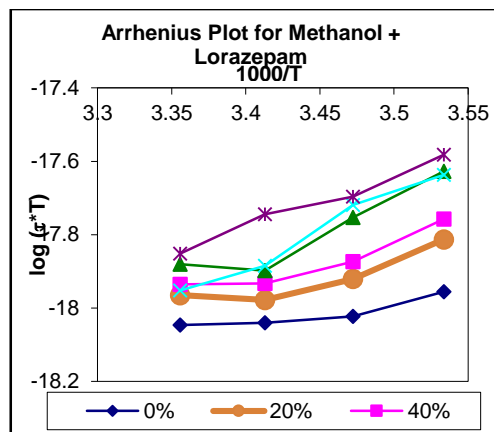

Figure 11. *Arrahenius plot of Lorazepam + Methanol Binary mixture.*

From figure 10, the growth in molar enthalpy of activation (ΔH) with volume fraction of Lorazepam in Methanol is observed. The growth from 4.069 KJ/mol up to 15.6KJ/mol, upto80% of Lorazepam in the mixture takes place. Further it is   decrease at12.05 KJ/mol (100% Lorazepam). For dipole reorientation the energy requirement is more up to 80% concentration of Lorazepam in the mixture, further for 100% concentration of Lorazepam in the mixture, energy requirement is becomes less [29]. Negative values of molar entropy of activation (ΔS) with volume fraction of Lorazepam indicate relatively high ordered arrangement of molecules in the activated state [30-32].

Arrhenius plot for the system is shown in fig 11. The Arrhenius plot is almost linear for this system. The raise in temperature causes raise in activation enthalpy (ΔH) shows straight characteristic of Arrhenius plot. The slope of Arrhenius plot shows the change in activation energy of the system with concentration. The state of need of temperature of relaxation time acts according with Arrhenius behavior [33, 34].

3.   CONCLUSION

The static dielectric constant (ε_s) and relaxation time (τ) obtained by fitting experimental statistics with the Debye equation. The static permittivity and relaxation time increases with increase in mole fraction and temperature of the system studied, indicating strong intermolecular interaction and molecules rotate easily. (ε_s)^E is positive for all .concentration indicate that there is increase in number of effective dipole and $(1/\tau)^E$ indicates rotation of the dipoles of the system. f$_B$ shows a deviation to upper side from the ideal Bruggeman behavior indicate effective volume of solvent gets enhanced in the presence of solute. The g^{eff} values more than 1 for all temperature, this indicates effective dipole become more as compare to pure liquid. This means that energy requirement is more

for group dipole reorientation. The Arrhenius plot is almost linear for this system. The Arrhenius behavior followed by temperature dependent relaxation time.

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