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TEMPERATURE DEPENDENT DIELECTRIC RELAXATION STUDY OF LORAZEPAM AND ETHANOL BINARY MIXTURE AT MICROWAVE FREQUENCY USING TIME DOMAIN REFLECTOMETRY TECHNIQUE

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Abstract: *The dielectric relaxation study for lorazepam and ethanol binary mixture has been carried out using the time domain reflectometry (T.D.R.) technique at temperature 283K, 288K, 293K and 298K and at different concentration, in the frequency range of 10MHz to 50Ghz. The dielectric parameters have been obtained from the complex permittivity spectra. The dielectric parameter shows change with temperature and concentration. The results obtained are used to interpret the nature and kind of solute-solvent interaction.*
Key words— *permittivity, relaxation time, excess properties, time domain reflectometry.*

Introduction

The dielectric relaxation study is one of the ways to obtain information regarding the solution. The chemicals used in the present work were ethanol and psychopharmaceutical drug lorazepam. Ethanol is a volatile, flammable, colorless liquid with a slight characteristic odor. The compound is widely used as a chemical solvent, either for scientific chemical testing or in synthesis of other organic compounds. [1]

Lorazepam is used to treat anxiety disorders and trouble sleeping. Due to its antagonistic effects on several receptor systems in the brain, lorazepam has anxiety-reducing effects. In the US, the FDA advises against use for longer than four weeks [2]

Physical constant of pure liquids Lorazepam and Ethanol

Name of Compound	Mol. Formula	Literature Value of ε_s	Mol. Wt. g/mol	Density in g/cm^3	Dipole Moment μ D
Lorazepam	$C_{15}H_{10}Cl_2N_2O_2$	NA	321.2	1.52	NA
Ethan	C_2H_5OH	24.5	46.	0.7	1.69

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II. Experimental

A. *Chemical and sample preparation*

The chemical used in the present work is lorazepam and ethanol is 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. These volume fractions are converted to mole fractions for further calculations. Using this volume percentage the weight fraction is calculated [3] 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 (Ethanol) respectively.

B. *T.D.R. specification,* Time domain *reflectometry set up and data acquisition.*

The Tektronix DSA8300 sampling oscilloscope sampling main frame with the dual channel sampling module 80E10B has been used for time domain reflectometry. The sampling module provides 12ps incident and 15ps reflected rise time pulse. The coaxial cable used to feed pulse has 50 Ohm impedance, inner diameter of 0.28mm and outer diameter of 1.19mm. Sampling oscilloscope monitors changes in pulse after reflection from end of line. Reflected pulse without sample $R_1(t)$ and with sample $R_x(t)$ were recorded in time window of 5 ns and digitized in 2000 points. To minimize the signal to noise ratio the signal reflected is obtained from 512 samples after an optimum average of 100 times for each record. The subtraction $[p(t) = R_1(t) – R_x(t)]$ and addition $[q(t) = R_1(t) + R_x(t)]$ of these pulses are done in oscilloscope memory. These subtracted and added pulses are transferred to PC through compact disc for further analysis. [4]

C. *Data analysis*

The time dependent data were processed to obtain complex reflection coefficient spectra, $\rho^*(\omega)$ over the frequency range from 10 MHz to 50 GHz using Fourier transformation [5,6] 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 is the velocity of light, ω is angular frequency and d is the effective pin length and j = root (-1). The complex permittivity spectra [7] $\varepsilon^*(\omega)$ were obtained from reflection coefficient spectra $\rho^*(\omega)$ by applying a bilinear calibration method. The experimental values of $\varepsilon^*(\omega)$ are fitted by Debye equation [8].

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

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_∞. A non-linear least squares fit method [9] used to determine the values of dielectric parameters.

III. Theory

A. *Excess permittivity and excess inverse relaxation time*

Information regarding to solute- solvent interaction may be obtained by excess properties [10] *i.e.* static dielectric constant and relaxation time in the mixtures. The excess permittivity is defined as [11]

$$\varepsilon_0^E = (\varepsilon_0)_m - [(\varepsilon_0)_A X_A + (\varepsilon_0)_B X_B] \quad (4)$$

Where, X is the mole fraction and the subscript m, A and B represent mixture, solute and solvent respectively. The excess permittivity provides qualitative information about multimer formation in the mixture as follows.

(i) ε^E=0: indicates that liquid A and liquid B do not interact and do not change their individual structural properties in the presence of other liquid.

(ii) $\varepsilon^E < 0$: indicates that liquid A and liquid B interact in such a way that the effective dipole moment gets reduced. The solute and solvent may form multimers leading to less effective diploes. In general the negative excess permittivity indicates the formation of multimers in the binary mixture.

(iii)$\varepsilon^E > 0$: indicates liquid A and liquid B interact in such a way that the effective diploe moment increases. This may be due to breaking of multimer structure into monomer structure in the presence of other molecule.

Similarly, the excess inverse relaxation time defined as

$$(1/\tau)^E = (1/\tau)_m - \left[(1/\tau)_A X_A + (1/\tau)_B X_B\right] \quad (5)$$

Where, $(1/\tau)^E$ is the excess inverse relaxation times, which represent the average broadening of dielectric spectra. Information regarding the dynamics of solute solvent interaction obtained from this excess property is as [12]

(i) $(1/\tau)^E = 0$: there is no change in the dynamics of liquid A and liquid B interaction,

(ii) $(1/\tau)^E < 0$: liquid A and liquid B interaction produces a field such that the effective dipoles rotate slowly,

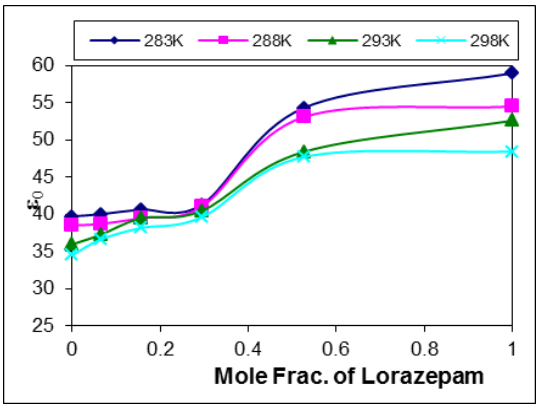
(iii) $(1/\tau)^E > 0$: liquid A and liquid B interaction produces a field such that the effective dipole rotate quickly, the field cooperate in rotation of dipoles.[13]

IV. Result and Discussion

A. *Permittivity and Relaxation Time*

Table: 1. Temperature dependent dielectric parameters for binary mixture of Lorazepam + Ethanol.

Mole Fraction of Lorazepam	283 K		288 K		293 K		298 K	
	ε_s	τ (ps)	ε_s	τ (ps)	ε_s	τ (ps)	ε_s	τ (ps)
0	39.71	171.6	38.54	152.2	35.96	139.5	34.48	127.8
0.0649	40.03	130.9	38.72	113.6	37.25	105.1	36.62	97.99
0.1562	40.63	111.2	38.49	96.75	39.46	91.17	38.16	76.26
0.2941	41.28	97.46	41.01	91.83	40.45	81.92	39.6	65.94
0.5262	54.31	95.58	53.08	80.99	48.4	74.01	47.71	59.16
1	58.96	81.78	54.47	61.66	52.58	57.13	48.43	47.27



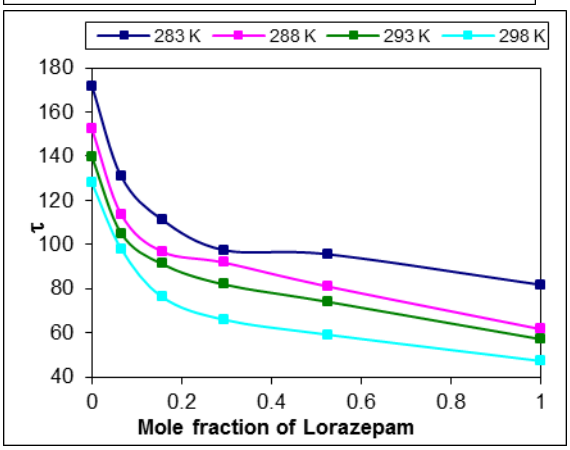


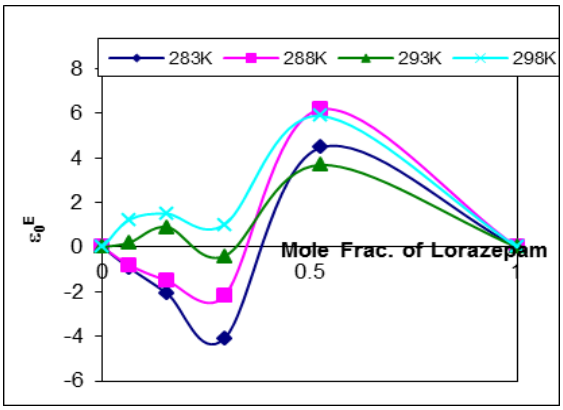
Figure 1: Variation of static dielectric constant (ε_s) as a function of mole fraction of Lorazepam at temperatures 283, 288, 293 and 298K.

Figure 2: Variation of relaxation time (τ) as a function of mole fraction of Lorazepam at temperatures 283, 288, 293 and 298K.

The static permittivity (ε_0) and relaxation time (τ) for the binary mixture obtained by fitting experimental data with the Debye equation at four different temperatures are shown in figs. 1 and 2 respectively. In this study, the variation in the static permittivity and relaxation time with lorazepam of ethanol are shown. It shows linear variation in the solution with change in mole fraction. This suggests that the intermolecular association is taking place in this region.

B. *Excess Permittivity and Excess Inverse Relaxation Time*

The variation of Excess permittivity (ε^E) and Excess inverse relaxation time with change in mole fraction of lorazepam at different temperatures is shown in fig (3) and (4)



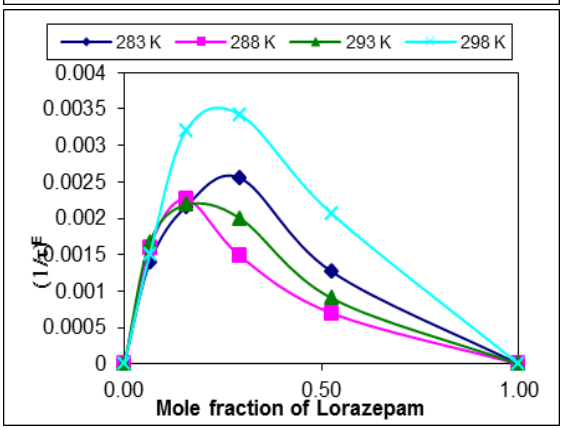


Figure 3: Variation of excess permittivity (ε_0^E) as a function of mole fraction (x_2) of lorazepam at 283, 288, 293 and 298K.

Figure 4: Variation of excess inverse relaxation time $(1/\tau)^E$, as a function of mole fraction (x_2) of lorazepam at 283, 288, 293 and 298K.

The variation of excess permittivity (ε_0^E) and excess inverse relaxation time $(1/\tau)^E$ with the mole fraction of lorazepam with ethanol at different temperature is shown in figs. 3 and 4. The excess permittivity (ε_0^E), values are positive after 40% of mole fraction of Lorazepam in ethanol at all temperature, This indicates change in alignment of dipole in the system due to increase in total number of dipoles.

The behavior in $(1/\tau)^E$ is quite different as can be seen from figure (4) the all values of $(1/\tau)^E$ are positive, but for lower concentration of lorazepam increases and then decreases at higher concentration at all temperatures. This suggests that at lower concentration of lorazepam the molecular interaction produces hindering field making effective dipole rotation slower. But at higher concentration of lorazepam the molecular interaction produces a cooperative field and the effective dipoles have more freedom of rotation.

V. Conclusion

The value of static permittivity (ε_0) increases with increasing concentration of lorazepam. It shows linear variation in dielectric constant. The values of relaxation time (τ) increases with increasing concentration of lorazepam. It shows linear variation in relaxation time with change in mole fraction. The excess permittivity (ε_0^E), values are somewhere positive and negative for different concentrations of lorazepam in ethanol at all temperature, positive at 80% and 100% of lorazepam and at 298K. This indicates change in alignment of dipole in the system, which increases total number of dipoles. The values of $(1/\tau)^E$ are positive, but for lower concentration of lorazepam it increases with decrease in concentration of ethanol and then decreases with increase in concentration of ethanol at all temperatures. This suggests that at lower concentration of

lorazepam the molecular interaction produces hindering field making effective dipole rotation slower. But at higher concentration it produces a cooperative field and the effective dipoles have more freedom of rotation.

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References:

1) https://en.wikipedia.org/wiki/Ethanol
2) http://en.wikipedia.org/wiki/Lorazepam
3) P. B. Undre, S.N.Helambe, S.B. Jagdale, P.W.Khirade and S.C. Mehrotra. Pramana J. Physics. 68. 851 (2007)
4) Manual T.D.R. Tektronix DSA8300
5) C. E. Shannon, Proc. Inst. Radio Eng. 37, 10(1949)
6) H.A. Samulan. Proc. IRE, 39, 175 (1951)
7) S. Mashimo, S. Kuwabara, S. Yogihara, and K. Higasi, J. Chem. Phy. 90, 3292(1989)
8) P. Debye. Polar Molecules, Chemical Catalog. Co. NewYork. (1929)
9) P. R. Bevington. Data Reduction and Error Analysis for the Physical Sciences, McGraw Hill, New York(1969)
10) Akl M. Awwad, Amar H. Al-Dujaili, and Salim R. Syriagh, J. Mol. Liq. 100(2), 129(2002)
11) S. C. Mehrotra and J.E Boggs, J. Chem. Phys. 66, 5306(1977)
12) S. B. Sayyad et al./ Lithuanian J. Phys. 51, 29-37 (2011)
13) http://shodhganga.inflibnet.ac.in/jspui/handle/10603/89385