

## Dielectric Relaxation Study of 2-Pentenenitrile and Chlorobenzene Molecules at 45<sup>o</sup>c Temperature

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### **Abstract:**

The time domain reflectometry (TDR) has been used for the study of dielectric relaxation spectra of 2-pentenenitrile (PN) and chlorobenzene (CBZ) binary mixtures. The frequency range for the study has been used as 10 MHz to 20 GHz. The system has been studied at 45<sup>o</sup>C temperature for 11 different concentrations. The dielectric parameters such as static permittivity ( $\epsilon_0$ ) and relaxation time ( $\tau$ ) have been obtained by Fourier transform and the least squares fit method. The relaxation in this system can be described by a single relaxation time using the Debye model. The Excess parameters such as excess permittivity and excess inverse relaxation time of the mixtures have been determined. In the mixtures excess permittivity ( $\epsilon^E$ ) is found positive. The excess inverse relaxation time ( $1/\tau^E$ ) is found negative. The investigation shows that the effective dipoles of the system increases. It also shows that due to the opposing field between the constituent molecules the dipole rotates slowly.

**Keywords:** Static Permittivity, Excess permittivity, Excess inverse relaxation time, TDR.

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### I. INTRODUCTION

The dielectric relaxation spectra study at microwave frequencies have been carried out to understand intermolecular and intramolecular interactions. Time Domain Reflectometer (TDR) is used to obtain the dielectric parameters of the system [1-3]. The dielectric relaxation parameters of binary mixtures give considerable information about solute-solvent interaction. It also provides the information about the charge distribution in a molecular system. Binary polar liquid consists of one associative and other non associative liquid. The liquid PN is of C $\equiv$ N group and CBZ of chlorine group. It is interesting to see the effect of nitrile group with chlorine-group. The frequency dependent complex permittivity measurements using TDR is more powerful technique because a single measurement covers a wide frequency range in a very short time. Several workers have studied the temperature dependent dielectric relaxation parameters. The objective of the present paper is to report the detailed study of dielectric relaxation for 2-pentenenitrile and chlorobenzene mixture using TDR at 45<sup>o</sup>C temperature at different 11 concentrations in the frequency range of 10MHz to 20GHz range.

### II. MATERIAL AND APPARATUS

A spectrograde 2-pentenenitrile (Fluka cheme GmbH-9471 Buchs, Steinheim, Switzerland) and AR grade chlorobenzene(CBZ) (E-Merck) were used without further purification. The solutions were prepared at 11 different volume percentages of PN in CBZ from 0 % to 100 % just before the measurements. Using these volume percents the mole fraction is calculated as

$$x_1 = (v_1\rho_1m_1) / [(v_1\rho_1m_1) + (v_2\rho_2m_2)]$$

Where  $m_i$ ,  $v_i$ , and  $\rho_i$  represent the molecular weight, volume percent, and density of the  $i^{\text{th}}$  ( $i=1, 2$ ) liquids, respectively. The density and molecular weight of the liquids are as follows:

2-Pentenenitrile(PN)- density:0.8329gmcm<sup>-3</sup>; mol.wt.-81.12

Chlorobenzene(CBZ)-density:1.1050gmcm<sup>-3</sup>;mol.wt.-112.56

The complex permittivity spectra were studied using the time domain reflectometry [4-5] method. The Hewlett Packard HP 54750 sampling oscilloscope with HP 54754A TDR plug in module has been used. A fast rising step voltage pulse of about 39 ps rise time generated by a pulse generator was propagated through a coaxial line system of characteristic impedance 50 Ohm. Transmission line system under test was placed at the end of coaxial line in the standard military applications (SMA) coaxial connector with 3.5 mm outer diameter and 1.35 mm effective pin length. All measurements were carried out under open load conditions. The change in the pulse after reflection from the sample placed in the cell was monitored by the sampling oscilloscope. In the experiment, time window of 5 ns was used. The reflected pulse without sample  $R_i(t)$  and with sample  $R_x(t)$  were digitized in 1024 points in the memory of the oscilloscope and transferred to a PC through 1.44 MB floppy diskette drive.

### III. DATA ANALYSIS

The time dependent data were processed to obtain complex reflection coefficient spectra  $\rho^*(\omega)$  over the frequency range from 10 MHz to 20 GHz using Fourier transformation [6, 7] as

$$\rho^*(\omega) = (c/j\omega d)[p(\omega)/q(\omega)] \quad (1)$$

Where  $p(\omega)$  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,  $\omega$  is angular frequency,  $d$  is the effective pin length and  $j = \sqrt{-1}$ .

The complex permittivity spectra  $\epsilon^*(\omega)$  were obtained from reflection coefficient spectra  $\rho^*(\omega)$  by applying bilinear calibration method [5].

The experimental values of  $\epsilon^*$  are fitted with the Debye equation [8]

$$\epsilon^*(\omega) = \epsilon_\infty + \frac{\epsilon_0 - \epsilon_\infty}{1 + j\omega\tau} \quad (2)$$

with  $\epsilon_0$ ,  $\epsilon_\infty$  and  $\tau$  as fitting parameters. A nonlinear least-squares fit method [9] was used to determine the values of dielectric parameters. In Eq.(2),  $\epsilon_0$  is the static dielectric constant,  $\epsilon_\infty$  is the limiting high-frequency dielectric constant and  $\tau$  is the relaxation time.

### IV. RESULTS AND DISCUSSION

The static dielectric constant ( $\epsilon_0$ ) and relaxation time ( $\tau$ ) obtained by fitting experimental data with the Debye equation are listed in Table 1. The values of static dielectric constant ( $\epsilon_0$ ) increases and relaxation time ( $\tau$ ) values have no specific trend with the increase of concentration of PN into CBZ.

The information related to liquids 1 and 2 interaction may be obtained by excess properties [10] related to the permittivity and relaxation times in the mixture. The excess permittivity  $\epsilon^E$  is defined as

$$\epsilon^E = (\epsilon_0 - \epsilon_\infty)_m - [(\epsilon_0 - \epsilon_\infty)_1 x_1 + (\epsilon_0 - \epsilon_\infty)_2 x_2] \quad (3)$$

Where  $x$ - mole fraction and suffices  $m$ , 1, 2 represents mixture, liquid 1 (PN) and liquid 2 (CBZ) respectively.

The excess permittivity may provide qualitative information about multimers formation in the mixture.

Similarly, the excess inverse relaxation time is defined as

$$(1/\tau)^E = (1/\tau)_m - [(1/\tau)_1 x_1 + (1/\tau)_2 x_2] \quad (4)$$

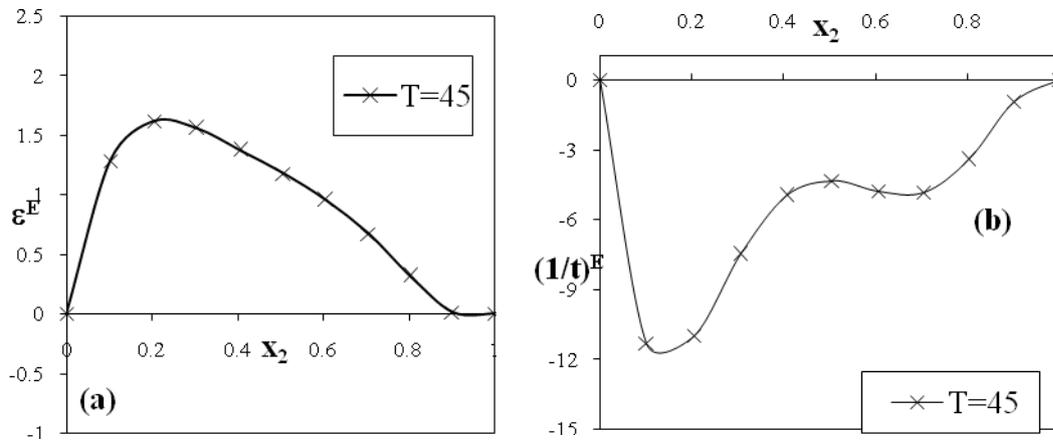
Where  $(1/\tau)^E$  is excess inverse relaxation time which represents the average broadening of dielectric spectra. The inverse relaxation time analogy is taken from spectral line broadening (which is inverse of the relaxation time) in the resonant spectroscopy [11].

The experimental values of both the excess parameters were fitted to the Redlich-Kister equation [12, 13]

$$A^E = (x_1 x_2) \sum_n B_n (x_1 - x_2)^n$$

Where  $A$  is either  $\epsilon^E$  or  $(1/\tau)^E$ . By using these  $B_n$  values,  $A^E$  values were calculated.

Figure 1, shows behavior of excess permittivity and excess inverse relaxation time for the system as a function of volume concentration of PN in CBZ at 45<sup>0</sup>C temperature.



**FIGURE1. (a)** The excess permittivity ( $\epsilon^E$ ) versus volume fraction of PN in CBZ  
**(b)** The excess inverse relaxation time  $(1/\tau)^E$  versus volume fraction of PN in CBZ.

**Table1:** Static dielectric constant ( $\epsilon_0$ ) and relaxation time ( $\tau$ ) for 45<sup>o</sup>C temperature.

Vol. percentage of PN in CBZ	$\epsilon_0$	$\tau$ (ps)
0	5.33(0)	13.01(0)
10	7.31(1)	15.65(8)
20	8.11(1)	13.46(6)
30	8.71(1)	14.3(11)
40	9.2(1)	12.87(14)
50	9.58(1)	12.48(12)
60	9.96(1)	12.16(12)
70	10.23(1)	12.52(9)
80	10.45(0)	11.57(5)
90	10.85(0)	11.36(9)
100		
	11.36(0)	10.98(0)

Number in bracket represent error in the corresponding value, e.g. means 12.16(12) means  $12.16 \pm 0.12$ .

In the system of PN-CBZ, from the excess permittivity ( $\epsilon^E$ ) curve we can see that the excess permittivity ( $\epsilon^E$ ) values are positives for all concentrations. The positive peak is obtained at 0.2049 concentrations. From positive peak the values are gradually decreases. The positive values indicates that; there is formation of monomeric or polymeric structures which leads to increase in total number of dipoles in the system. It also shows parallel alignment of the dipoles.

The excess inverse relaxation time ( $1/\tau^E$ ) values are negatives for all concentration. The negative peak is obtained at 0.1028 concentrations. From the peak point to pure PN the values are decreases continuously. The negative values of ( $1/\tau^E$ ) indicates that; the effective dipoles in the system creates hindering field. It also represents that; the effective dipole rotation becomes slowly.

## V. CONCLUSION

The dielectric parameters such as dielectric constant and relaxation time values of 2-pentenenitrile (PN) and chlorobenzene (CBZ) mixtures are obtained by analyzing dielectric relaxation spectra. The excess permittivity and excess inverse relaxation time values are also reported for 11 different concentrations at 45<sup>o</sup>C temperature in the frequency range of 10 MHz to 20 GHz. This data provides information regarding solute-solvent interaction. From the present study we conclude that; the total number of dipoles in the system increases and the parallel alignment of the dipoles in the PN-CBZ system. We also conclude that; the dipoles produces opposing field in the mixture and rotates slowly.

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