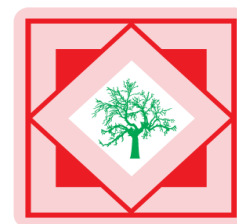




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### 150°C Temperature dependent dielectric relaxation study of pentanenitrile and 1,2-dichloroethane mixture

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#### ABSTRACT

The dielectric relaxation spectra of pentanenitrile(PN) and 1,2 Dichloroethane(DCE) mixture has been studied at 15<sup>0</sup>C temperature in the frequency range of 10 MHz to 20 GHz using time domain reflectometry (TDR) for 11 different concentrations of the system. 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 Excess parameters of the mixtures such as excess permittivity and excess inverse relaxation time have been determined. In the mixtures excess permittivity ( $\epsilon^E$ ) is found to be positive. The excess inverse relaxation time  $(1/\tau)^E$  is found to be negative. It indicates that the effective dipoles produces hindering field in the mixture and dipole rotates slowly.

**Keywords:** Nitrile group, Chloro group, Dielectric parameters, Excess permittivity, Excess Inverse relaxation time, Time Domain Technique.

**PACS:** 77.22

#### INTRODUCTION

The information of molecular interaction between the constituent molecules of the mixture can be obtained by the study of dielectric spectra. Time Domain Reflectometry (TDR) was used to study the dielectric spectra of the system [1-2]. It also provides the information about the charge distribution in a molecular system. It is interesting to see the effect of PN as nitrile group with DCE as chlorine-group. The objective of the present paper is to study the dielectric relaxation of pentanenitrile and 1, 2-Dichloroethane mixture using TDR at 15<sup>0</sup>C temperature at different 11 concentrations for the frequency range of 10MHz to 20GHz range. The dielectric parameters such as dielectric constant and relaxation time for the binary mixtures have also been determined.

#### MATERIALS AND APPARATUS

A spectrograde butanenitrile (Fluka cheme Gmbh-9471 Buchs, Steinheim, Switzerland) and AR grade 1,2 Dichloroethane (E-Merck) were used without further purification. The solutions were prepared at 11 different volume percentages of BN in DCE 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:

Butanenitrile- density: 0.8329 gm cm<sup>-3</sup>; mol.wt.-67.09,

1,2-Dichloroethane-density:1.256gmcm<sup>-3</sup>;mol.wt.-98.96

The complex permittivity spectra were studied using the time domain reflectometry [3] 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  $R_1(t)$  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.

#### 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 [4, 5] 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 [3].

The experimental values of  $\epsilon^*$  are fitted with the Debye equation [6]

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

With  $\epsilon_0$ ,  $\epsilon_\infty$  and  $\tau$  as fitting parameters. A nonlinear least-squares fit method [7] 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.

#### 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 the relaxation time ( $\tau$ ) values have no specific trend.

Figure 1, (a) shows behavior of excess permittivity for the system as a function of volume concentration of PN in DCE at 15°C temperature and (b) shows behavior of excess inverse relaxation time for the system as a function of volume concentration of PN in DCE at 15°C temperature.

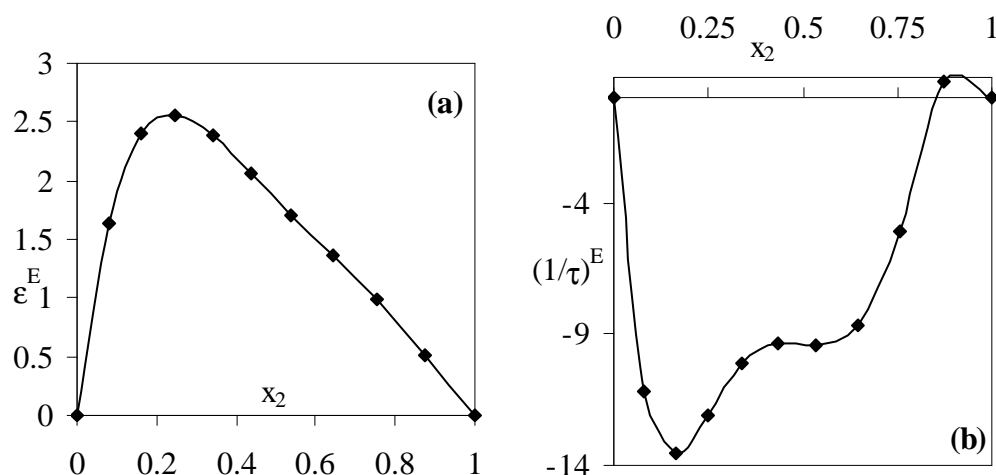


FIGURE 1. (a) The excess permittivity ( $\epsilon^E$ ) versus volume fraction of PN in DCE.  
 (b) The excess inverse relaxation time  $(1/\tau)^E$  versus volume fraction of PN in DCE.

The information related to liquids 1 and 2 interaction may be obtained by excess properties [8] 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 (DCE) 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 [9].

The experimental values of both the excess parameters were fitted to the Redlich-Kister equation [10, 11]

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

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

The excess permittivity ( $\epsilon^E$ ) values are positive for all concentrations. The excess permittivity ( $\epsilon^E$ ) increases sharply towards the peak values then decreases slowly up to pure PN. In the PN-DCE system excess permittivity ( $\epsilon^E$ ) curve, the peak value is noted at 0.2486 mole fraction of PN in DCE. Then it shows that there is a linear decrease up to pure PN. Hence there is formation of monomeric or polymeric structures. The total effective dipole increases. It shows a parallel alignment of dipoles.

The excess inverse relaxation time values are negatives except 0.87.42 concentrations. It also shows that there is sudden increase in  $(1/\tau)^E$  from 0 to 0.1618 concentration of PN and it decreases to pure PN. The negative values of inverse relaxation time indicate that; the effective dipoles produce an opposing field in the molecules and the slower effective dipole rotation of the molecules in the system.

Table1: Static dielectric constant ( $\epsilon_0$ ) and relaxation time ( $\tau$ ) for 15°C temperature.

| Volume percentage of PN in DCE | $\epsilon_0$ | $\tau$ (ps) |
|--------------------------------|--------------|-------------|
| 0                              | 10.88        | 11.46       |
| 10                             | 13.64        | 13.48       |
| 20                             | 14.7         | 13.89       |
| 30                             | 15.93        | 13.92       |
| 40                             | 16.73        | 13.9        |
| 50                             | 17.68        | 13.67       |
| 60                             | 17.96        | 14.59       |
| 70                             | 18.82        | 14.4        |
| 80                             | 19.58        | 13.65       |
| 90                             | 20.42        | 13.42       |
| 100                            | 21.14        | 13.66       |

## CONCLUSION

The dielectric parameters such as static permittivity, relaxation time are reported. The dielectric constant increases as the concentration of PN increases in DCE. The values of excess permittivity and excess inverse relaxation time are also reported for pentanenitrile and 1, 2-dichloroethane system at 15°C temperature for 11 different concentrations. The excess permittivity graph shows that the effective dipole increases. The negative values of  $(1/\tau)^E$  indicate that there is a formation of hindering field in the molecules of the mixture and the dipole rotates slowly.

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