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Relaxation study of pentanenitrile and 1, 2-dichloroethane mixtures at 25⁰C temperature

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ABSTRACT

The dielectric relaxation spectra of pentanenitrile (PN) with 1,2 Dichloroethane (DCE) mixture at temperature 25⁰C in the frequency range of 10 MHz to 20 GHz using time domain reflectometry (TDR) for 11 different concentrations of the system have been studied. The dielectric parameters such as static permittivity and relaxation time for the mixture have been reported. The excess dielectric constant and excess inverse relaxation time have also studied. The investigation shows that the effective dipoles increases and the dipoles rotates slowly due to the hindering field between the constituent molecules of the PN and DCE mixture.

Keywords: Relaxation time, Dielectric parameters, Nitrile group, Chloro group, Time Domain Reflectometer.
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INTRODUCTION

The relaxation of the molecules in the mixture study at microwave frequencies gives intermolecular interactions and also shows dynamics of the molecules of the liquid mixtures using time domain reflectometry [1-2]. Pentanenitrile (PN) is non-associative liquids and 1, 2 Dichloroethane (DCE) is associative liquid. PN is nitrile group and DCE is of chlorine group. It is interesting to see the effect of nitrile group with chlorine-group. The objective of the present paper is to study the formation about monomers and multimers between molecules of pentanenitrile and 1, 2 Dichloroethane mixtures at 25⁰C temperature.

MATERIALS AND METHODS

A spectrograde pentanenitrile (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 PN in DCE from 0 % to 100 % just before the measurements. Using these volume percents the mole fraction is calculated as

$$x_1 = (v_1\rho_1/m_1) / [(v_1\rho_1/m_1) + (v_2\rho_2/m_2)]$$

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

Pentanenitrile- density: 0.795 gmcm⁻³; mol. wt. - 81.12

1,2Dichloroethane-density: 1.256 gmcm⁻³; mol. wt. - 98.96

The complex permittivity spectra were studied using the time domain reflectometry [3-4] 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 [5, 6] 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, ω 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 [4].

The experimental values of ϵ^* are fitted with the Debye equation [7]

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

With ϵ_0 , ϵ_∞ and τ as fitting parameters. A nonlinear least-squares fit method [8] was used to determine the values of dielectric parameters. In Eq. (2), ϵ_0 is the static dielectric constant, ϵ_∞ is the limiting high-frequency dielectric constant and τ is the relaxation time.

RESULTS AND DISCUSSION

The static dielectric constant (ϵ_0) and relaxation time (τ) obtained by fitting experimental data with the Debye equation are listed in Table 1. The values of static dielectric constant (ϵ_0) increases and relaxation time (τ) values initially increases and then decreases with the increase of concentration of PN into DCE.

Figure 1(a) Shows behavior of excess permittivity and (b) the excess inverse relaxation time for the system as a function of volume concentration of PN in DCE at 25°C temperature

(b) The excess inverse relaxation time $(1/\tau)^E$ versus volume fraction of PN into DCE.

The information related to liquids 1 and 2 interaction may be obtained by excess properties [9] related to the permittivity and relaxation times in the mixture. The excess permittivity ϵ^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 [10].

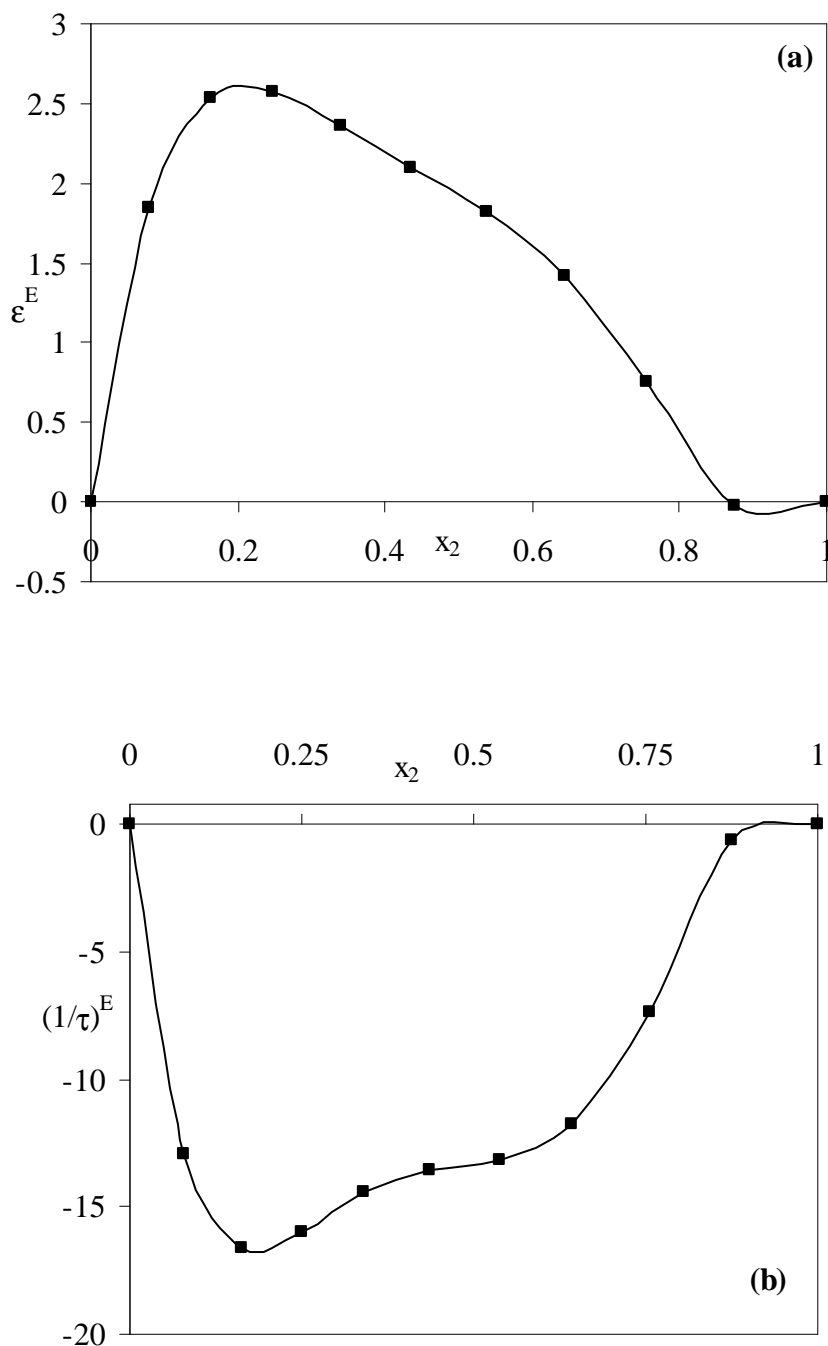


FIGURE 1.(a)The excess permittivity (ϵ^E) versus volume fraction of PN into DCE.

The experimental values of both the excess parameters were fitted to the Redlich-Kister equation [11, 12]

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

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

The excess permittivity (ϵ^E) increases sharply towards the peak values then decreases slowly and goes also in the negative region up to pure PN. In the PN-DCE system excess permittivity (ϵ^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. The value goes in negatives from concentration 0.8742. The ϵ^E values are positive in DCE rich region. Hence there is formation of monomeric or polymeric structures. The total effective dipole increases. There is a parallel alignment of dipoles in DCE rich region. The values of excess permittivity are negatives in PN rich region. It indicates that there is decrease in dipole of the mixture. Hence there is anti parallel alignment of dipoles in PN rich region.

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

Table1: Static dielectric constant (ϵ_0) and relaxation time (τ) for 25°C temperature.

Volume percentage of PN	ϵ_0	τ (ps)
0	10.43	10.7
10	13.05	12.98
20	14.59	13.26
30	15.85	13.48
40	16.34	13.7
50	17.05	13.63
60	17.9	14.48
70	18.65	13.9
80	19.29	13.28
90	19.55	13.01
100	21	13

CONCLUSION

The dielectric parameters such as static dielectric permittivity and relaxation time have been reported for PN-DCE mixtures at 25°C temperature for 11 different concentrations. The excess dielectric parameters are also obtained. The values of excess permittivity are positives and it indicates that; the effective dipoles form monomers and increases. The excess inverse relaxation times are negative and it shows that; the dipoles in the mixture form opposing field and dipole rotates slowly.

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