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# Interaction of Butanenitrile with 1,2-dichloroethane using Microwaves at 25$^o$C

I.G. Shere[a]

[a]*Department of Electronics, Shri Havagiswami Mahavidyalaya,Udgir-413 517, India*

***Abstract***

*The dielectric relaxation spectra have been studied for 1, 2-dichloroethane with butanenitrile mixtures in the frequency range of 0.1 GHz to 20 GHz using time domain reflectometry (TDR) at 25$^o$C temperatures for 11 different concentrations of the system. The dielectric parameters viz. static dielectric constant ($\varepsilon_0$) and relaxation time ($\tau$) have been obtained by the least squares fit method. Kirkwood correlation factor and effective Kirkwood correlation factor of the mixtures have been determined. The static dielectric constants for the mixtures have been fitted with the modified Bruggeman model.*

***Keywords-*** *Butanenitrile, 1,2-dichloroethane, binary mixture, dielectric properties, TDR.*

## I. INTRODUCTION

Dielectric relaxation study of liquid mixture gives information about molecular interaction. Considerable dielectric relaxation study has been done in chloro group with alcohol group [1]. In this work, the report of the dielectric study of 1, 2-dichloroethane-butanenitrile mixture has been given. The butanenitrile (BN) is a non-associative liquid and 1, 2 dichloroethane (DCE) is an associative liquid, one with C≡N and other with chloro group. It is interesting to see the effect of BN in chloro-group.

In present paper an attempt has been made to study the molecular interaction between associative with non-associative liquids of the mixture at different concentrations and temperatures.

## II. EXPERIMENTAL

A spectrograde butanenitrile 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

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

where $m_i$, $v_i$, and $\rho_i$ represent the molecular weight, volume percent, and density of the i$^{th}$ (i=1, 2) liquids, respectively.

The complex permittivity spectra were studied using the time domain reflectometry [2-5] 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 50Ω. 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 $R_l(t)$ 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.

The temperature controller system with water bath and a thermostat has been used to maintain the constant temperature within the accuracy limit of ±1$^o$C. The sample cell is surrounded by a heat insulating container through which the water of constant temperature using a temperature controller system is circulated. The temperature at the cell is checked using the electronic thermometer.

## III. DATA ANALYSIS

The time dependent data were processed to obtain complex reflection coefficient spectra $\rho^*(\omega)$ over the frequency range from 0.1 GHz to 20 GHz using Fourier transformation [6, 7] as

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

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 $\varepsilon^*(\omega)$ were obtained from reflection coefficient spectra $\rho^*(\omega)$ by applying bilinear calibration method [2].

The experimental values of ε* are fitted with the Debye equation [8]

$$\varepsilon^*(\omega) \quad = \quad \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 + j\omega\tau} \qquad (2)$$

with $\varepsilon_{0,}$ $\varepsilon_\infty$, and $\tau$ as fitting parameters. A nonlinear least-squares fit method [9] was used to determine the values of dielectric parameters. In Eq. (2), $\varepsilon_0$ is the static dielectric constant, $\varepsilon_\infty$ is the limiting high-frequency dielectric constant and $\tau$ is the relaxation time. The value of $\varepsilon_\infty$ was taken to be 2 for the system studied, for the frequency range considered here, $\varepsilon^*$ is not sensitive to $\varepsilon_\infty$.

## IV. RESULTS AND DISCUSSION

The static dielectric constant ($\varepsilon_0$) and relaxation time ($\tau$) obtained by fitting experimental data with the Debye equation. This value shows the behavior of static dielectric constant of DCE-BN system, as a function of mole fraction of BN in DCE at 25$^o$C temperature and 11 concentrations.

The value of static dielectric constant increases with increasing the mole fraction of BN and relaxation time increases up to 10% volume of BN and then it becomes decreases for increasing concentrations of BN in DCE for the system.

The Kirkwood correlation factor g [10] is also a parameter for getting information regarding orientation of electric dipoles in polar liquids. The $g_f$ for pure liquid may be obtained by the expression

$$\frac{4\Pi N\mu^2\rho}{9kTM}g = \frac{(\varepsilon_0-\varepsilon_\infty)(2\varepsilon_0+\varepsilon_\infty)}{\varepsilon_0(\varepsilon_\infty+2)^2} \qquad (3)$$

where $\mu$ is dipole moment in gas phase, $\rho$ is density at temperature T, M is molecular weight, k is Boltzman constant, N is Avogadro's number. The dipole moments for DCE and BN in gas phase are taken as 1.83 D and 3.91 D [11] respectively.

For the mixture of two polar liquids 1, 2 Eq. (3) is modified by ref. [12] with the following assumptions:

1. Assume that g for the binary mixture is expressed by an effective averaged correlation factor $g^{eff}$ such that the Kirkwood equation for the mixture can be expressed by

$$\frac{4\Pi N}{9kT}\left(\frac{\mu_1^2\rho_1}{M_1}\phi_1+\frac{\mu_2^2\rho_2}{M_2}\phi_2\right)g^{eff} = \frac{(\varepsilon_{0m}-\varepsilon_{\infty m})(2\varepsilon_{0m}+\varepsilon_{\infty m})}{\varepsilon_{0m}(\varepsilon_{\infty m}+2)^2} \qquad (4)$$

with $\phi_1$ and $\phi_2$ as volume fractions of liquids 1 and 2 respectively.

2. Assume that the correlation factors for molecules 1 and 2 in the mixture contribute to the effective g proportionality to their pure-liquid values $g_1$, $g_2$. Under this assumption the Kirkwood equation for the mixture can be written

$$\frac{4\Pi N}{9kT}\left(\frac{\mu_1^2\rho_1 g_1}{M_1}\phi_1+\frac{\mu_2^2\rho_2 g_2}{M_2}\phi_2\right)g_f = \frac{(\varepsilon_{0m}-\varepsilon_{\infty m})(2\varepsilon_{0m}+\varepsilon_{\infty m})}{\varepsilon_{0m}(\varepsilon_{\infty m}+2)^2} \qquad (5)$$

where $g^{eff}$ is the effective Kirkwood correlation factor for a binary mixture, with $\phi_1$ and $\phi_2$ as volume fractions of liquids 1 and 2 respectively.

In equation (4), the values of $g^{eff}$ will change from $g_1$ to $g_2$ as concentration of molecule 2 will decrease from 100% to 0%. The Kirkwood correlation factor $g_f$, which gives angular correlation between the molecules of the system, is less than 1. This indicates that the effective dipoles in the mixture will be less than the corresponding average value in pure liquids.

The values of $g^{eff}$ and $g_f$ are calculated from equation (4) and (5) are given in Table I for the mixtures of the system. Errors are also estimated by assuming 2 % error in the values of the permittivity.

The effective values of the correlation factor for DCE are larger than the corresponding value in BN. The value of $g^{eff}$ increase for 10% then there is linear decrease with increase of the % of BN in the system. These values less than one indicate antiparallel orientation of the electric dipoles in the system. The values of $g_f$ deviate maximum from unity. The maximum deviation from unity is observed around 50% of BN in DCE mixture. The values of $g^{eff}$ and $g_f$ for the system are shown in Figure I.

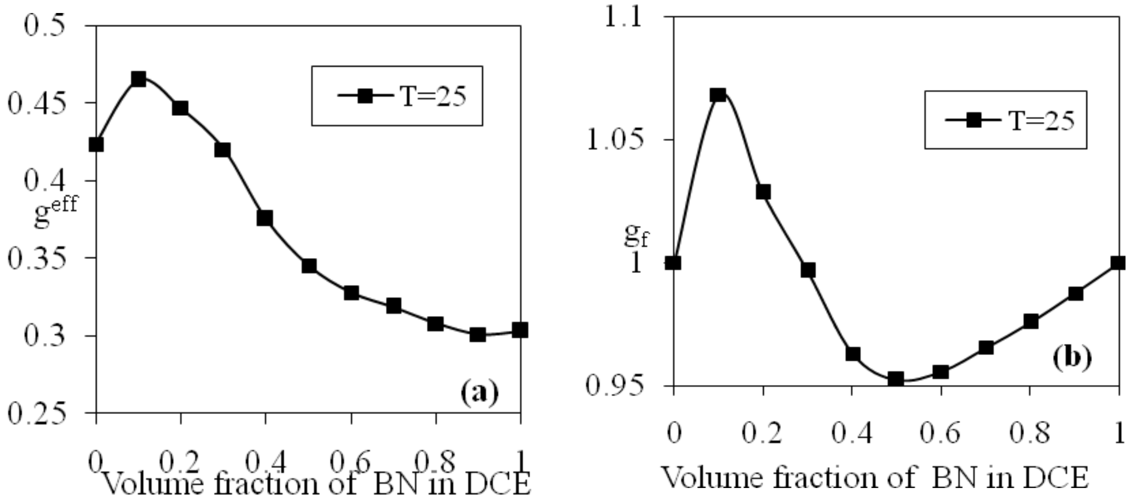

**Figure I.** a) Effective Kirkwood factor b) Kirkwood factor

The modified Bruggeman equation [13] is another parameter, which may be used an indicator of liquid 1 and 2 interaction. The Bruggeman factor $f_B$ is given by,

$$f_B = \left(\frac{\varepsilon_{0m}-\varepsilon_{02}}{\varepsilon_{01}-\varepsilon_{02}}\right)\left(\frac{\varepsilon_{01}}{\varepsilon_{0m}}\right)^{1/3} = (1-\phi_2) \qquad (6)$$

According to equation (6), a linear relationship is expected which will give a straight line when plotted $f_B$ against $\phi_2$. However, here the experimental values of $f_B$ were found to deviate from the linear relationship. The Bruggeman dielectric factor $f_B$ versus volume fraction $\phi_2$ of BN at 25°C is given in Figure 2.

To fit the experimental data, Eq. (6) has been modified [14].

$$f_B=1-[a-(a-1)\phi_2]\phi_2 \qquad (7)$$

where 'a' is numerical fitting parameter.

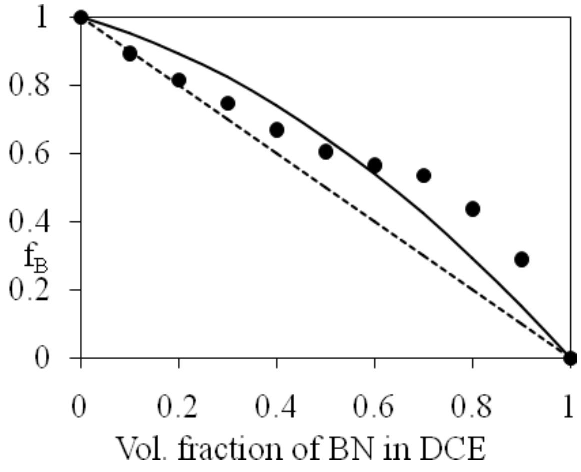

**Figure 2.** The Bruggeman plot for BN-DE mixture at 25$^o$C.Dashed line denote original model (equation 9).Continuous line is the theoretical curve obtained from equation (10).Experimental points are shown by the symbol •.

The parameters ‘a’ has been determined by the least squares fit method and it is found to be 0.415 for temperature 25. The value of ‘a’ = 1 corresponds to the ideal Bruggeman mixture formula. The deviation from 1 relates to corresponding liquids 1 and 2 interactions. The large deviation of “a” suggest that strong interaction and small between DCE and BN.

## V. CONCLUSION

Dielectric relaxation parameters and Kirkwood parameters have been reported for DCE-BN mixtures at 25$^0$C temperature and 11 concentrations. This data provide information regarding solute-solvent interaction in liquids. The $g^{eff}$ values decreases linearly with increase in concentration of BN in the solution.

The values of Kirkwood correlation factor indicates the intermolecular interactions of the chloro group with the C≡N bonded liquids. The dielectric behavior of this binary mixture is found to agree with the modified Bruggeman equation. It shows strong interaction between the constituent molecules.

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