

Temperature Dependence Dielectric Relaxation Study of Aqueous 1, 3-Butanediol using TDR.

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Abstract:

The Complex dielectric spectra $\epsilon^*(\omega)=\epsilon'-j\epsilon''$ of binary mixture of 1, 3-Butanediol with water were obtained in the microwave frequency range 10 MHz to 30 GHz using Time Domain Reflectometry (TDR) technique. The static dielectric constant (ϵ_0) and relaxation time (τ) have been obtained at different temperatures. On the basis of dielectric parameters intermolecular interaction are predicated.

Keywords: Time domain, complex dielectric spectra, Relaxation time. Temperature.

done on diol-water mixtures using time domain reflectometry [9].

In this paper the systematic dielectric relaxation studies of 1,3-butanediol in water solutions at different concentrations at different temperatures have been carried out using time domain reflectometry technique from 10MHz to 30GHz. The dielectric study such as complex permittivity spectra, static dielectric constant, relaxation time, dielectric loss, thermodynamic properties of each concentration of 1,3-butanediol in water solutions have been evaluated.

I. Introduction:

1,3-butanediol (1,3-BD) is the organic compound having structural formula $\text{OHCH}_2\text{CH}_2\text{CHOHCH}_3$, this colorless liquid is derived from butane alcohol groups at first and third carbon of the chain. It is commonly used as a solvent for food flavoring agents and is a comonomer used in certain polyurethane and polyester resins. 1,3-Butanediol is a highly effective humectants in pet foods, tobacco and cosmetic formulations. They are clear viscous liquids that are miscible with water and most polar organic solvents. The physical and chemical properties of the butanediols make them suitable as organic solvents and useful chemical intermediates in the manufacture of many chemical products. The environment of water solvent can be modified by the diol molecules because of strong interactions between the hydroxyl group and water. Extensive dielectric relaxation studies were carried out for different concentrations of a diol-water system to understand the solute-solvent interactions and dynamic behavior of water [1-6]. The associating behavior and the frequency dependences of complex permittivity for 1,3-BD and in water mixture are extensively studied through dielectric properties and cooperative domains [7]. The time domain reflectometry (TDR) is very useful technique to study the dielectric relaxation parameters of liquids [8]. This technique covers a broadband of frequencies in a single measurement. In our laboratory the considerable dielectric work has been

II. Experimental Method and Data

Analysis:

The dielectric spectra were obtained by the time domain reflectometry (TDR) technique. The Tektronix model no. DSA8200 Digital Serial Analyzer sampling mainframe along with the sampling module 80E08 has been used for the time domain reflectometry (TDR). A repetitive fast rising voltage pulse with 18ps incident rise time was fed through coaxial line system of impedance 50 ohm. Sampling oscilloscope monitors changes in step pulse after reflection from the end of line. Reflected pulse without sample $R_1(t)$ and with sample $R_x(t)$ were recorded in time window of 2ns and digitized in 2000 points. The time dependent data were processed to obtain complex reflection coefficient spectra $\rho^*(\omega)$ over the frequency range from 10 MHz to 30 GHz as [2, 3, 10].

$$\rho^*(\omega) = \left(\frac{c}{j\omega d} \right) \left[\frac{p(\omega)}{q(\omega)} \right]$$

where $p(\omega)$ & $q(\omega)$ are Fourier transforms of $[R_1(t)-R_x(t)]$ and $[R_1(t)+R_x(t)]$ respectively, c is the speed of light, ω is the angular frequency, d is the effective pin length and $j=\sqrt{-1}$. The complex permittivity spectra $\epsilon^*(\omega)$ was obtained from reflection coefficient $\rho^*(\omega)$ by applying calibration method as described earlier [4]. The dielectric permittivity ϵ' and dielectric loss ϵ'' of 1,3-Butanediol with water at different temperatures are

shows complex permittivity spectra for 1,3-Butanediol-water mixtures at different temperatures respectively as a function of frequency from 10 MHz to 30 GHz. It is observed from the plot that values of ϵ' decreases with increase in concentration

of 1,3-BD and maxima of the dielectric loss ϵ'' maximum shifts from the higher to lower frequency range.

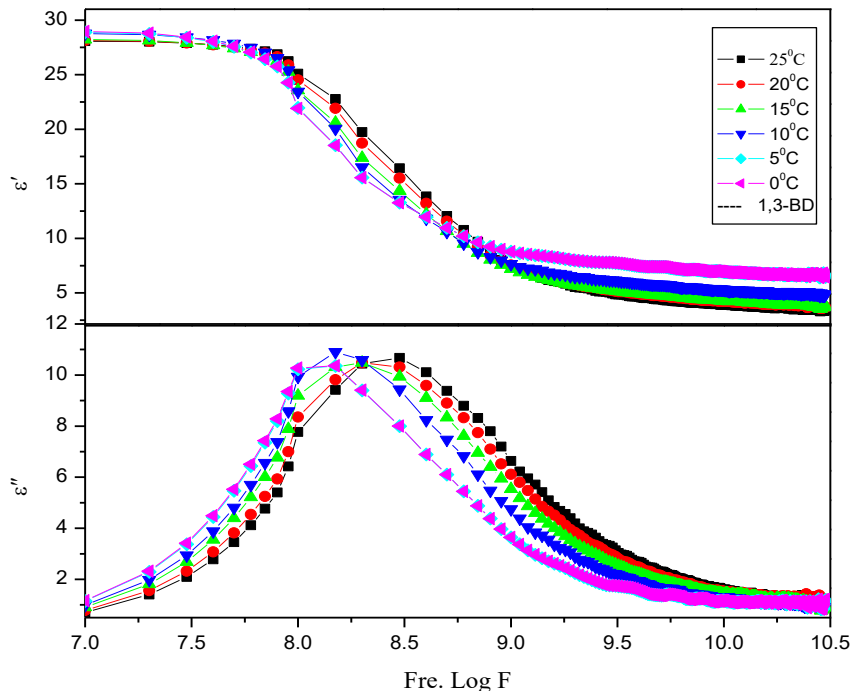


Figure: Complex permittivity spectra (ϵ' & ϵ'') of 1,3-BD at different temperatures.

III. Result and Discussion:

The general form of the dielectric relaxation model is given by the Havriliak-Negami equation [11-13].

$$\epsilon^*(\omega) = \epsilon_\infty + \frac{(\epsilon_0 - \epsilon_\infty)}{[1 + (j\omega\tau)^{(1-\alpha)}]^\beta}$$

where ϵ_0 is the static permittivity, ϵ_∞ is the permittivity at high frequency, τ is the relaxation time, α and β are the empirical parameters for the distribution of relaxation times with values between 0 and 1. The Havriliak-Negami equation includes three relaxation models as limiting forms. The Debye model ($\alpha = 0$ and $\beta = 1$) implies a single relaxation time while the Cole – Cole model ($0 \leq \alpha \leq 1$ and $\beta = 1$) and Cole-Davidson ($\alpha = 0$ and $0 \leq \beta \leq 1$) both suggest a distribution of relaxation times. The magnitudes of α and β indicates the width of the distribution. The aqueous solutions of 1,3BD volume percentage concentrations of BDs could fit

Cole-Davidson type dispersion. Therefore, here $\alpha=0$ and $0 \leq \beta \leq 1$ and experimental values of $\epsilon^*(\omega)$ were fitted to the Cole-Davidson equation as,

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

Where the values of ϵ_0 , τ & ϵ_∞ are fitting parameter. A non-linear least squares fit method was used to determine the values of dielectric parameters. The values of $\epsilon_0, \epsilon_\infty$ & τ (ps) for pure 1,3-butanediol at different temperatures as in Table. The errors in the last significant digits are also reported. The values of static dielectric constant and relaxation time are increases with decrease in temperature in 1,3-BD. The smaller values are found in 1,3-BD, this is may be due to the position of -OH group in BD as reported by Bozena S. & Karol.[14]

Table: Dielectric relaxation parameters of 1,3-Butanediol at different temp.

System	Temp.	ϵ_0	τ (ps)	ϵ_∞	β
1,3-BD	25 ⁰ C	28.23(14)	546.37(858)	2.93(1)	0.80(3)
	20 ⁰ C	30.42(18)	588.32(116)	3.36(1)	0.77(4)
	15 ⁰ C	30.65(18)	682.01(131)	3.50(1)	0.77(4)
	10 ⁰ C	31.41(21)	800.05(179)	4.60(1)	0.72(5)
	5 ⁰ C	32.33(28)	1042.33(327)	6.20(1)	0.73(6)
	0 ⁰ C	32.44(28)	1050.89(330)	6.21(1)	0.73(6)

Thermodynamic Properties:

The thermodynamic parameters evaluated using Eyring equation is as follows.

$$\tau = (h/KT) \exp (\Delta H/RT) \exp (-\Delta S/R)$$

Where ΔS are the entropy of activation, ΔH is the activation energy in kJ/mole. τ is the relaxation time in PS and T is the temperature in K and h is the Planck constant. The result in values of activation energy and entropy of activation of 1, 3-Butanediol are obtained by least square fit method are reported in Table. The value of activation energy of 1, 3-BD. This suggests that hydrogen bonding in 1, 3-BD is stronger. The temperature dependence of relaxation time described by Arrhenius plot for Pure 1,3-Butanediol have been shown Straight line.

Table: Thermodynamic Properties of 1,3-Butanediol.

System	$\square H$ (kJ/mole)	$\square S$ (j/mole k)
1,3-Butanediol	17.52(1)	0.22

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