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Molecular Interaction study of Multi-Functional Group of Alcohols through Dielectrics Using TDR

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Abstract. The complex permittivity spectra for tert-butyl alcohol(TB) with n-propanol(nP) were determined over the frequency range of 10 MHz to 20 GHz using the time domain reflectometry (TDR) in the temperature range of 25°C to 55°C for 11 different concentrations of the system. The static dielectric constant (ϵ_0) and relaxation time (τ) have been determined these spectra using the Debye model. Excess properties and Kirkwood correlation factor of the mixtures have been determined. The excess permittivity is found to be positive in the tert-butyl alcohol rich region and negative in the n-Propanol rich region. However, the excess inverse relaxation time has different trend. The static dielectric constants for the mixtures have also been fitted with the modified Bruggeman model by assuming an additional parameter in the model.

1. Introduction

The measurement and characterization of the response of a material to an applied electric field is called dielectric analysis. Dielectric analysis measures changes in the properties of a material as it is subjected to a periodic electric field. The dielectric relaxation of binary polar liquids provides information regarding their interactions. In this work, we report the dielectric study of tert-butyl alcohol (TB) with n-propanol (nP) mixture; both are hydroxyl group molecules.

2. Experimental

TB and nP (AR grade, Merck Pvt. Ltd., West Mumbai, India) were used without further purification. The solutions were prepared at 11 different volume percentage of nP in TB from 0 % to 100 % in steps of 10 %. 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:

TB: Density=0.8093 gmcm⁻³, Mol. Wt. = 74.12

nP : Density= 0.7997 gmcm⁻³, Mol. Wt. = 60.11

The complex permittivity spectra were studied using the time domain reflectometry [1]-[6] method. The Hewlett Packard HP 54750 sampling oscilloscope with HP 54754A TDR plug in module has been

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used. The temperature controller system with water bath and a thermostat has been used to maintain the constant temperature within the accuracy limit of $\pm 1^\circ\text{C}$.

3. 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 [7], [8] 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 experimental values of $\epsilon^*(\omega)$ are fitted with the Debye equation [9]

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

with ϵ_0 , ϵ_∞ and τ as fitting parameters. A nonlinear least-squares fit method [10] was used to determine the values of dielectric parameters.

4. Results and Discussion

The obtained values of ϵ_0 , ϵ_∞ and τ are listed in Table 1. 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(TB) and liquid 2(nP) respectively.

The excess permittivity may provide qualitative information about multimers formation in the mixture as follows: $\epsilon^E = 0$, the liquid 1 and 2 do not interact; $\epsilon^E < 0$, the liquid 1 and 2 interaction in such a way that the total effective dipoles get reduced and $\epsilon^E > 0$, indicates the liquid 1 and 2 interaction such that the total effective dipole moment increases.

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 in the resonant spectroscopy [12]. The information regarding the dynamic of liquid 1 and 2 interactions from this excess property is as: $(1/\tau)^E = 0$; there is no change in the dynamics of liquid 1 and 2 interaction, $(1/\tau)^E < 0$; the liquid 1 and 2 interaction produces a field such that the effective dipoles rotate slowly and $(1/\tau)^E > 0$; the liquid 1 and 2 interaction produces a field such that the effective dipoles rotate quickly.

The experimental values of both the excess parameters were fitted to the Redlich-Kister equation [13], [14] as

$$A^E = (x_1 x_2) \sum_n B_n (x_1 - x_2)^n \quad (5)$$

where A is either ϵ^E or $(1/\tau)^E$. By using these B_n values, A^E values were calculated. The 'g' values for pure liquid may be obtained by the expression

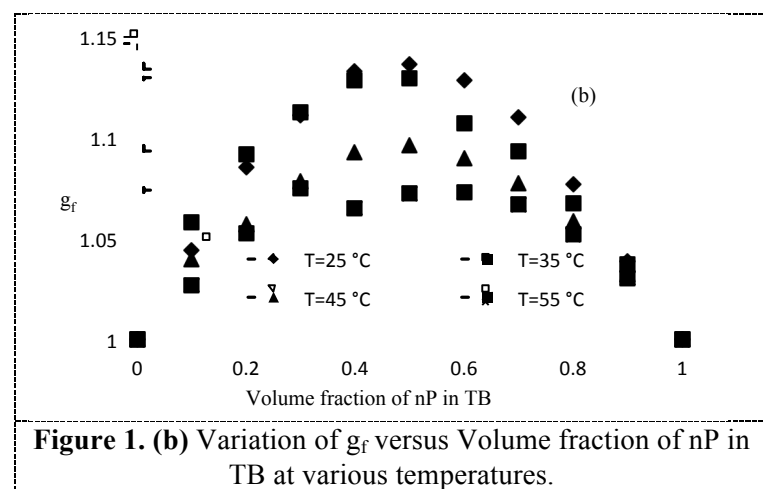
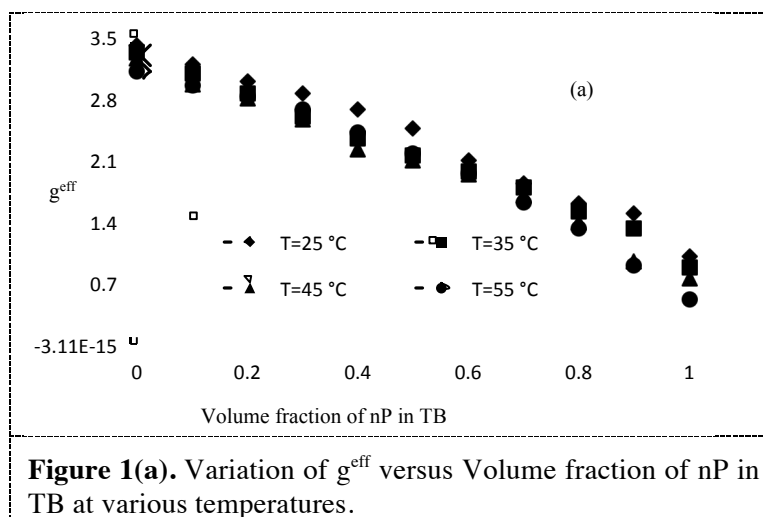
$$\frac{4\pi N\mu^2 \rho}{9kTM} g = \frac{(\epsilon_0 - \epsilon_\infty)(2\epsilon_0 + \epsilon_\infty)}{\epsilon_0(\epsilon_\infty + 2)^2} \quad (6)$$

where μ is dipole moment in gas phase, ρ is density, M is molecular weight, k is Boltzmann's constant and N is Avogadro's number. The dipole moments for TB and nP in gas phase are taken as 1.69 D and 1.68 D respectively [15]. Temperature dependent g^{eff} and g_f for the system is also shown in Fig. 1, (a) and (b).

Table 1. Temperature Dependent Dielectric Relaxation Parameters for TB + NP mixture*

x_2	T= 25 °C	T= 35 °C	T= 45 °C	T= 55°C
ϵ_0				
0.0000	11.89(0)	11.32(0)	10.87(0)	09.34(0)
0.1197	15.06(4)	13.87(9)	12.62(3)	10.99(1)
0.2342	16.54(2)	14.50(7)	13.27(5)	11.40(2)
0.3439	17.69(3)	15.39(2)	13.97(2)	11.97(4)
0.4492	18.24(7)	16.03(2)	14.70(8)	12.55(2)
0.5502	18.89(3)	17.36(3)	15.52(4)	13.17(4)
0.6473	19.54(9)	18.03(4)	16.26(5)	13.84(1)
0.7406	20.02(2)	18.60(9)	16.92(9)	14.97(3)
0.8303	20.73(7)	19.29(3)	17.60(8)	15.53(4)
0.9167	21.28(3)	19.89(2)	18.47(4)	16.15(1)
1.0000	21.94(0)	20.18(0)	19.02(0)	16.83(0)
ϵ_∞				
0.0000	3.26(1)	3.09(0)	2.80(0)	2.61(1)
0.1197	2.89(4)	2.74(1)	2.70(3)	2.50(0)
0.2342	2.65(3)	2.59(3)	2.55(4)	2.39(3)
0.3439	2.38(8)	2.34(8)	2.29(8)	2.14(4)
0.4492	2.08(2)	2.01(4)	2.01(3)	1.98(7)
0.5502	1.86(7)	1.81(2)	1.86(9)	1.79(2)
0.6473	1.64(9)	1.59(1)	1.60(7)	1.52(8)
0.7406	1.54(4)	1.38(9)	1.32(2)	1.28(3)
0.8303	1.33(3)	1.18(3)	1.08(4)	1.04(1)
0.9167	1.27(8)	0.97(4)	0.89(3)	0.81(4)
1.0000	0.81(0)	0.78(0)	0.69(0)	0.63(0)
τ (ps)				
0.0000	0.0000	0.0000	0.0000	0.0000
0.1197	0.1197	0.1197	0.1197	0.1197
0.2342	0.2342	0.2342	0.2342	0.2342
0.3439	0.3439	0.3439	0.3439	0.3439
0.4492	0.4492	0.4492	0.4492	0.4492
0.5502	0.5502	0.5502	0.5502	0.5502
0.6473	0.6473	0.6473	0.6473	0.6473
0.7406	0.7406	0.7406	0.7406	0.7406
0.8303	0.8303	0.8303	0.8303	0.8303
0.9167	0.9167	0.9167	0.9167	0.9167
1.0000	1.0000	1.0000	1.0000	1.0000

* x_2 is the mole fraction of nP in TB. Number in bracket represent error in the corresponding value.



5. Conclusion

The study has provided the permittivity parameters for the mixture of binary polar liquids. The molecules of these compounds have several hydrogen bonding sites and enter into intra or inter molecular hydrogen bonding giving rise to different conformations. This provides a unified approach to understand the interaction between two constituents in the liquid mixtures, using different models.

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