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Title:	Disruption of the self-molecular association of pentanol in binary mixtures with alkylbenzoates: a dielectric relaxation spectroscopy study
Authors:	Begum, S. (/jspui/browse?type=author&value=Begum%2C+S.) Vardhan, Abhinay (/jspui/browse?type=author&value=Vardhan%2C+Abhinay) Chaudhary, Atul (/jspui/browse?type=author&value=Chaudhary%2C+Atul) Subramanian, R. (/jspui/browse?type=author&value=Subramanian%2C+R.)
Keywords:	Pentanol Spectroscopy Dielectric Alkylbenzoates
Issue Date:	2016
Publisher:	Royal Society of Chemistry
Citation:	RSC Advances, 6(2), pp. 1260-1267
Abstract:	The disruption of the self-molecular association of pentanol by the presence of alkylbenzoate was studied using dielectric relaxation spectroscopy. The complex permittivity spectra of binary mixtures of pentanol (1-pentanol, 2-pentanol and 3-pentanol) and alkylbenzoate (methylbenzoate, ethylbenzoate, propylbenzoate and butylbenzoate) for the entire composition range were determined in a frequency range of 200 MHz to 20 GHz using a vector network analyzer at room temperature. The raw data were fitted to the Havriliak–Negami equation to evaluate the various dielectric parameters of static dielectric constant (ϵ_s), high frequency limiting dielectric constant (ϵ_∞), and relaxation time (τ). The non-linear behaviour of these parameters for mixtures with a pentanol mole fraction represents the hetero-association of polar solvent molecules. A complex of alkylbenzoate with 2-pentanol and 3-pentanol has lower number of dipoles in solution than 1-pentanol and thus, there is a decrease in the molar volume of the rotating entity. The relaxation time reflects that the reorientation of the –OH group of 1-pentanol in a binary mixture with alkylbenzoate is more pronounced than it is for 2-pentanol and 3-pentanol. The dielectric parameters were used in calculating the excess permittivity, excess inverse relaxation time, Kirkwood correlation factor, and Bruggeman factor. These dielectric results were used in interpreting the molecular interaction of the binary mixture with different dipoles in the liquid state.
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