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Title:Onset of hydrogen bonded collective network of water in 1,4-dioxane
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Abstract:We have studied the evolution of water hydrogen bonded collective network dynamics in mixtures of 1,4-dioxane (Dx) as the mole fraction of water (X w) increases from 0.005 to 0.54. The inter- and intramolecular vibrations of water have been observed using terahertz time domain spectroscopy (THz-TDS) in the frequency range 0.4 - 1.4 THz (13 - 47 cm-1) and Fourier transform infrared (FTIR) spectroscopy in the far-infrared (30 - 650 cm-1) and mid-infrared (3000 - 3700 cm-1) regions. These results have been correlated with the reactivity of water in these mixtures as determined by kinetic studies of the solvolysis reaction of benzoyl chloride (BzCl). Our studies show an onset of intermolecular hydrogen bonded water network dynamics beyond XW >; 0.1. At the same concentration, we observe a rapid increase of the rate constant of solvolysis of BzCl in water - Dx mixtures. Our results establish a correlation between the onset of collective hydrogen bonded network with the solvation dynamics and the activity of clustered water. (Figure presented)
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