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标题: Hydration Shell Parameters of Aqueous Alcohols: THz Excess Absorption and Packing Density
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摘要: Solvation in water requires minimizing the perturbations in its hydrogen bonded network. Hence solutes distort water molecular motions in a surrounding domain, forming a molecule-specific hydration shell. The properties of those hydration shells impact the structure and function of the solubilized molecules, both at the single molecule and at higher order levels. The size of the hydration shell and the picoseconds time-scale water dynamics retardation are revealed by terahertz (THz) absorption coefficient measurements. Room-temperature absorption coefficient at f = 0.28 [THz] is measured as a function of alcohol concentration in aqueous methanol, ethanol, 1,2-propanol, and 1-butanol solutions. Highly diluted alcohol measurements and enhanced overall measurement accuracy are achieved with a THz absorption measurement technique of nL-volume liquids in a capillary tube. In the absorption analysis, bulk and interfacial molecular domains of water and alcohol are considered. THz ideal and excess absorption coefficients are defined in accordance with thermodynamics mixing formulations. The parameter extraction method is developed based on a THz excess absorption model and hydrated solute molecule packing density representation. First, the hydration shell size is deduced from the hydrated solute packing densities at two specific THz excess absorption nonlinearity points: at infinite alcohol dilution (IAD) and at the THz excess absorption extremum (EAE). Consequently, interfacial water and alcohol molecular domain absorptions are deduced from the THz excess absorption model. The hydration shell sizes obtained at the THz excess absorption extremum are in excellent agreement with other reports. The hydration shells of methanol, ethanol, 1- and 2-propanol consist of 13.97, 22.94, 22.99, and 31.10 water molecules, respectively. The hydration shell water absorption is on average 0.774 +/- 0.028 times the bulk water absorption. The hydration shell parameters might shed light on hydration dynamics of biomolecules.
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