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标题: Urea, a Structure Breaker? Answers from THz Absorption Spectroscopy
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摘要: There has been a controversial debate of whether urea can be regarded as structure breaker or a structure maker. Here, we present concentration and temperature dependent absorption coefficients of urea water mixtures in the THz. range (1.5-10 THz, 50-350 cm(-1)). Our results are in agreement with the hypothesis that urea adapts ideally into the, water network. Using a semi-ideal chemical association model and accompanying MD simulations, the observed spectra. could be decomposed in three contributions: one is attributed to hulk water, a second one to rattling modes of weakly solvated urea in the surrounding water cage, and the third part accounts for THz modes describing a doubly hydrogen bonded strong solvent-solute interaction. The bands attributed to the rattling motion of the solute scale linearly with concentration. The intensity of this contribution is temperature independent in contrast to the water and strongly solvated solute absorption We find that. even at high urea concentrations the Majority of water retains a bulklike absorption spectrum, whereas only a small number (about 0.5-1.1 per urea on average). are strongly bound in the temperature range between 9 and 36 degrees C. The THz absorption data provide no evidence for urea aggregation in the concentration range investigated (1-10 M).
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