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Title: Intermolecular vibrational mode of the benzoic acid dimer in solution observed by terahertz time-domain spectroscopy
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Abstract: The low-frequency modes of the benzoic acid (BA) dimer and its analogues in carbon tetrachloride (CCl(4)) have been investigated by terahertz time-domain spectroscopy. The solute spectrum is obtained by subtracting the solvent contribution from that of the solution. The difference spectrum of BA in CCl(4) has a broad band with a peak at 68 cm(-1). To assign the observed band, the spectrum is compared with spectra of other aromatic molecules, such as benzene and phenol in addition to p-methyl BA and deuterated BA species (BA-d(OH) and BA-d(5)) in CCl(4). The band at 68 cm(-1) is assigned to the cogwheel mode of the BA dimer. Density functional theory calculations also support this assignment. Finally, spectral lineshape analysis based on the multimode Brownian oscillator model is applied to the THz spectra for all the samples.