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Terahertz Spectroscopy of Hydrogen-Bonded Molecular Complexes in Solution TIMOTHY KORTER, ANNA JOSEPH, Syracuse University — Hydrogen bonding is ubiquitous in nature and governs a wide array of chemical and biological processes. Although the hydrogen bond is well studied, its low-frequency vibrations – the large-amplitude motions involving stretching and bending along the actual hydrogen-bond coordinates – have been rarely investigated. These vibrations largely fall in the terahertz (THz) or far-infrared region (0.1-6 THz). Here we present pulsed THz spectroscopic investigations of intermolecular hydrogen bonding in several molecular clusters in non-aqueous solutions. In order to access spectral data above 3 THz, a pulsed THz spectrometer utilizing gallium phosphide (GaP) crystals was constructed to provide >6 THz of continuous spectral bandwidth. Molecular systems to be discussed include the mixed dimeric systems of phenol:pyridine and 4-fluorophenol:pyridine, as well as the phenol trimer. Experiments will also be presented on the 7- azaindole dimer which serves a model system for the phenomenon of excited- state double-proton transfer. In all cases, density functional theory calculations were used to assign the observed vibrational features to specific vibrational motions of the complexes. Finally, preliminary optical-pump-THz-probe experiments concerning the excited-state dynamics of these molecular complexes will be discussed.

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