CW THZ SPECTROSCOPY OF SMALL PEPTIDES

K. SIEGRIST, D. F. PLUSQUELLIC, *National Institute of Standards and Technology, Gaithersburg MD 20899 USA*; R. BALU, S. GREGURICK, *Dept. of Chemistry and Biochemistry, University of Maryland, Baltimore, MD 21250*; I. MANDELBAUM, A. R. HIGHT WALKER, *National Institute of Standards and Technology, Gaithersburg MD 20899 USA.*

CW THz spectroscopy has been used to investigate the lowest frequency vibrational modes of small peptides. Due to their non-local character, these large amplitude modes are remarkably sensitive to intermolecular hydrogen bonding. THz spectra obtained from 2 cm^{-1} to 100 cm^{-1}, for three different crystalline forms of alanine tripeptide at 4.2 K were all quite different. These three forms included one parallel and two anti-parallel beta sheet structures. The latter two forms differ only in the presence and absence of water molecules that bridge and cross link the sheets. Despite the weak nature of the water hydrogen bonds, the THz spectra for the hydrated and dehydrated antiparallel structures of trialanine are drastically different, while spectra observed for the two forms in the mid-infrared region were indistinguishable. Together with data obtained at intermediate hydration levels, these results provide insight into the nature and scope of forces fields necessary to model these low energy interactions. Spectral predictions obtained for crystal-like structures using the CHARMM force field and for various dimer forms from density functional theory will be discussed.