Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Developing a Vibrational Spectral Maker for Probing the Hydrogen Bonding Status of Buried Asp and Glu Residues AIHUA XIE, BEINING NIE, JERROD STUTZMAN, Oklahoma State University, AIHUA XIE TEAM — Hydrogen bonding is a fundamental element in protein structure and function. Breaking a single hydrogen bond may impair the stability of a protein. We report an infrared vibrational spectral marker for probing the hydrogen bond number for buried, protonated Asp or Glu residues in proteins. Ab initio computational studies were performed on hydrogen bonding interactions of a COOH group with a variety of side chain model compounds of polar and charged amino acids in vacuum using density function theory. In addition, we show an approximate linear correlation between the C=O stretching frequency and the hydrogen-bond strength. We propose that a two-dimensional infrared spectroscopy, C=O stretching vs. O-H stretching, may be employed to identify the specific type of hydrogen bonding interaction. This vibrational spectral marker for hydrogen bonding interaction is expected to enhance the power of time-resolved Fourier transform infrared spectroscopy for structural characterization of functionally important intermediates of proteins.

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Date submitted: 07 Dec 2004 Electronic form version 1.4