

CONFORMATION SPECIFIC SPECTROSCOPIC INVESTIGATION OF β - and α/β -PEPTIDES: INSIGHT INTO THE AMIDE I AND AMIDE II SPECTRAL SIGNATURES

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β -peptides differ from naturally occurring α -peptides in having an extra carbon linking amide groups in the polypeptide chain. β - and α/β -peptides, while not as extensively studied as their α -peptide analogs, have recently been shown to have quite diverse, diagnostic spectral signatures in the amide NH stretch region of the infrared spectrum. While these spectra have provided a basis for assignment to particular hydrogen bonded architectures, extension of these studies of conformation specific infrared spectra into the mid-infrared would be particularly useful, since amide carbonyl stretch and amide NH bend transitions can provide complementary insight to the nature of the hydrogen bonding involved. This talk will present the spectral signatures of small β - and α/β -peptides in the Amide I and Amide II spectral regions, 1200-1800 cm^{-1} . Additionally, the experimental results will be compared with DFT and *ab initio* results to aid in the understanding of the spectral signatures and as benchmark examples of the requirements for theory to quantitatively describe infrared spectra in this spectral range.