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UV Resonance Raman Excitation Profiles and Depolarization Ratios of Peptide Conformations BHAVYA SHARMA, SANFORD ASHER, University of Pittsburgh — UV resonance Raman spectroscopy is a well established technique for probing peptide and protein secondary structure. Excitation between 180 to 215 nm, within the π to π* electronic transitions of the peptide backbone, results in the enhancement of amide vibrations. We use UVRR excitation profiles and depolarization ratios to examine the underlying peptide bond electronic transitions. The present consensus is that three electronic transitions (n to π* and two π to π*) occur in simple amides between 230 and 130 nm. In α-helices a weak n to π* electronic transition occurs at 220 nm, while a higher frequency π to π* transition occurs at 190 nm. This π to π* transition undergoes exciton splitting, giving rise to two dipole-allowed transitions: one perpendicular to the helical axis (190 nm) and the second parallel to the axis (205 nm). The melted state of alpha-helices resembles left-handed poly-proline II (PPII) helices. The PPII helix electronic transitions have been defined as an n to π* transition at $\sim$ 220 nm and a π to π* transition at $\sim$ 200 nm. For beta-sheets, the π to π* transition occurs at $\sim$ 194 nm for parallel and $\sim$196 nm for anti-parallel sheets. n to pi* transition occurs at $\sim$217 nm for both.

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