Dependence of polyproline ROA on the peptide length

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Polyproline-II helical conformation (PPII) represents a less common protein secondary structure. Its structure is rather specific because there are no internal stabilizing hydrogen bonds in it. The rigidity of the helix is caused only by sterical reasons and the interaction with surrounding solvent molecules. Number of recently discovered evidence [1] has lead to a presupposition that the PPII helix is the main element of the random-coil protein structure. This information provides a new reason to study PPII conformation and specifically problematic of its formation, which has not been thoroughly studied yet.

In our experiment we measured Raman and Raman optical activity (ROA) spectra of several oligo- and poly-L-proline samples in a wide frequency range between 120 cm^{-1} and 1800 cm^{-1} and analyzed them with respect to the length of the proline chain. The relatively new technique of ROA [2,3], which is based on a different interaction of a specimen with the right- and left-handed circularly polarized laser light, represented an ideal methodology for this type of observation due to its high sensitivity to the conformational stability and rigidity of peptide chain backbone. There is also a strong link to previous experiments [4] which were focused on the characterization of proline side chain conformation and its interaction with solvent.

So far, we were able to determine the characteristic spectral peaks associated with formation of stable PPII helical conformation in studied systems. The most relevant peaks are located at 405, 535 and 945 cm^{-1}. Moreover, based on our experimental data analysis we were able to determine the minimal length of $(\text{L-proline})_N$ chain necessary for creation of the stable PPII conformation as N=6 [5].

The stress is laid on the interconnection between experimental and theoretical approach. For that purpose we perform *ab initio* calculations of ROA spectral bands and their intensities for all measured samples in order to obtain more accurate interpretation of recorded spectra and observed phenomena.

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