Hydrogen-bond cooperativity, vibrational coupling, and dependence of helix stability on changes in amino acid sequence in small 3_{10}-helical peptides. A density functional theory study.

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Streszczenie

Five pentapeptides, GGGGG, GAGGG, GVGGG, GLGGG, and GIGGG, have been completely optimized in the 3_{10}-helical and open β-strand conformations at the B3LYP/D95** level. The energies of the helices relative to the β-strands vary from −2.1 to −3.6 kcal and depend on the amino acid residue sequence. The energies of substituting A, V, L, or I for G in the second position are also presented. Vibrational analyses were performed on the optimized structures. Vibrational coupling through the individual H-bond chains of the helices is confirmed to be stronger than that through space or through the covalent bonds. The cooperative interactions of the H-bonds are evident from both the structures and the coupling of the amide I, amide II, and N−H vibrations.

Słowa kluczowe

Amides, Chemical structure, Energy, Oscillation, Peptides and proteins

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