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The quantum-chemical modeling of peptide hydrogen bonds in dimer of glycin

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Abstract

The study of the nature of hydrogen bonds in biologically active and medicinal substances is topical. The instability of the hydrogen bond can significantly affect the state of pharmaceuticals containing, for example, amino acids during their long-term storage, transportation or processing. One of the methods for studying nature and determining the strength of hydrogen bonds is quantum-chemical modeling. In this paper modeling of the α-glycine dimer was carried out within the framework of the theory of the self-consistent reaction field by the DFT/B3LYP/6-31G(d,p) method with complete geometry optimization without symmetry constraints. Theoretical spectra were obtained on the basis of the results of calculation of the force field in the harmonic approximation. The results of the calculation were visualized in the ChemCraft program. In the theoretical Raman spectrum only low-frequency (2500 cm^{-1}) vibrations of hydrogen N-H...O bonds of two molecules are due to vibrations of the hydrogen bond. Calculations show the peculiarity of such a hydrogen bond: when the hydrogen bond is preserved, N-H breaks and O-H forms. In the 3200-3500 cm^{-1} region there are four lines, each of which corresponds to stretching vibrations of free N-H bonds of the amino group of one molecule. The calculation of the interaction energy in the investigated associate and its decomposition were carried out using the Morokuma method (HF/6-31G (PC GAMESS)). It is established that all the components contribute significantly to the interaction energy of the two glycine molecules, with the exception of the mixing energy. Taking into account the superposition error of the basic set, the value of the BSSE interaction energy is -58.28 kcal/mol and corresponds to two strong hydrogen bonds. It does not contradict the data on the crystal structure of α-glycine.

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