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Theoretical calculations are a strong tool in the investigation of strong intramolecular hydrogen bonds

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Streszczenie

This chapter deals with strong intramolecular hydrogen bonds. Strong intramolecular hydrogen bonds are complicated to describe on the basis of quantum chemistry methods. They are short and easily modified by external factors, e.g. the substituent effects in the parent molecule, or solvent effects. Calculation of energies is clearly very important in assessing the intramolecular hydrogen bond. Several schemes have been suggested. One way is to calculate the energy difference between the hydrogen-bonded and the open form, also called "closed and open", and use this as a theoretical measure of the hydrogen bond energy. Historically, infrared spectroscopy has been the most important spectroscopic method in the study of hydrogen bonding, and the possibility to predict the vibrational transitions of hydrogen-bonded systems by theoretical calculations has been of great interest for decades. Principal component analysis has been used to analyze deuterium ^{13}C isotope effects and ^{13}C nuclear magnetic resonance chemical shifts in Schiff bases.

Słowa kluczowe

hydrogen bond energy, infrared spectroscopy, intramolecular hydrogen bonds, nuclear magnetic resonance calculations, principal component analysis, solvent effects, vibrational transitions

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