

Computational Studies of Hydrogen–Bonds in Nucleobases

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Hydrogen–bonds interactions are very important especially to make 3D shapes of biological compounds. Since the pioneering work of Watson and Crick to characterize the structures of DNA, considerable efforts have been dedicated to explore the mysteries insides the nucleobases structures.^{1,2}The nucleobases could contribute to hydrogen–bond interactions with other nucleobases or polar molecules. Water molecules are also very important part of these interactions in biological media. In addition to the original nucleobases, the hydrogen–bonds interactions are also important in their derivatives, which mainly have pharmaceutical applications e.g., fluorouracil. Therefore, characterizations of hydrogen–bonds interactions are very important regarding their important roles in biological systems. *Ab initio* computational methods based on density functional theory are the proper approach to investigate the properties of hydrogen–bonded systems. Optimization processes for singular molecules in the isolated gas phase could yield insightful information about their natural properties in the absence of any perturbation and interactions. Moreover, the effect of interactions around the central molecule could be very well investigated through optimization calculations based on first principles methods. The computed parameters obtained by atomic scale spectroscopic techniques e.g., NMR, could also reveal important aspects of hydrogen–bonded systems. Since the strengths of hydrogen–bonds are not so much as covalent bonds, high–level computations are proper tools to achieve the purpose of investigating their properties especially for the nucleobases.

1. J.D. Watson, F.H.C. Crick, A structure for deoxyribose nucleic acid; *Nature* 171 (1953) 737.
2. M. Mirzaei, O. Gülseren, N. Hadipour, DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs; *Comput. Theor. Chem.* 1090 (2016) 67.

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