The influence of the number of π electrons on hydrogen bonds in Adenine-Thymine and derivative systems

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Abstract

The number of π electrons in the pair Adenine-Thymine (AT) has been the basis of the study in order to know their influence on hydrogen bonds. The work has been developed by using DFT approach (BLYP/TZ2P) and by using also smaller structures than the original nucleobases.

We have done a quantitative energy decomposition analysis for hydrogen bonds to study whether binding energy changes when making the skeleton smaller. Moreover, an analysis of Voronoi deformation density (VDD) method is used to show changes in charges. In addition, gaps between the σ donor-acceptor interacting orbitals and σ orbital interaction energy contribution for each hydrogen bond will be also relevant features.

With the analyses we have studied whether π-electrons of the non-interacting atoms play an important role when forming the two hydrogen bonds of AT. We have observed that π polarization contributes with a small magnitude on hydrogen bonds and resonance assisted hydrogen bonds (RAHB) linked with the π delocalization has been questioned in favour of σ contributions.

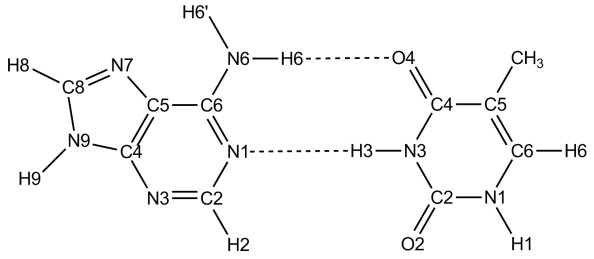

Figure 1: Adenine-Thymine with the nomenclature used.