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Effects of hydration on the base pair structures of guanine: Stacked vs. planar base pairing

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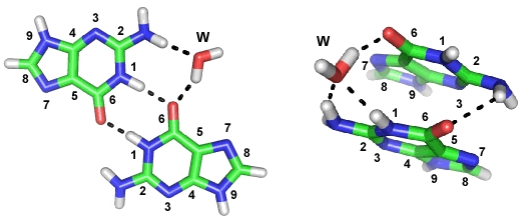
The three-dimensional structure of DNA is stabilized mainly by hydrogen-bonding and stacking interactions between the nucleic acid bases. In addition, the degree of hydration plays a key role in the secondary and tertiary structure. However, it is difficult to elucidate how the solvation affects the conformation of DNA by separating from the base pair interactions. Studying isolated DNA base pairs enables us to investigate pairing and stacking interactions in the absence and presence of water molecules. Most theoretical calculations suggested that upon addition of water molecules, stacked structures of the base pairs are stabilized with respect to the planar hydrogen-bonded base pairs.
In this work, we have investigated the effects of microhydration on the stabilization of guanine-guanine (GG) and guanine-cytosine (GC) base pairs by the ab initio MP2, MP4(SDQ), and CCSD methods. In the case of the GG pair, the stability of a specific stacked structure is increased by the addition of a water molecule, being nearly isoenergetic to the planar base pair having symmetric double hydrogen-bonding. One the other hand, two most stable monohydrate structures obtained for the GC pair are those of the Watson-Crick (WC) base pair. Monohydrated structures associated with the stacked GC pair are found to be low in energy. The larger stability of the monohydrate obtained for the stacked GG pair can be explained by the difference in the binding energy of the stacked structure between the GG and GC pair. The overlap of the two aromatic planes may be larger for the stacked GG pair than for the GC pair. Although the present result suggests that stacked base pairs are significantly stabilized by the hydration, no experimental evidence for the stacked monohydrates has been obtained.

Low-energy monohydrates of the GG base pair



Planar Stacked