

Hydrogen Bonding Interactions in Stacked Watson-Crick and Mismatched DNA Base Pairs

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We have theoretically analyzed a complete series of stacked Watson-Crick and mismatched DNA base pairs, both in gas phase and in water. We show that the twist angle between the two base pairs appears to be determinant with respect to the strength of the stacking interaction, and cause an energy gain on the order of 7 kcal mol⁻¹. The stacked base pairs with the most unfavorable stacking interaction at 0° appear to be those that are methyl substituted (thymine or difluorotoluene), although the stacking improves considerably at the experimental twist angle (36°) due to the reduction of steric repulsion. On the other hand, the diagonal interactions present between the stacked bases are shown to play a very important role with respect to the overall stabilization of these stacked complexes. Finally, the larger stability of GC-rich DNA compared to AT-rich DNA is highlighted.