Abstract

Hydrogen bonding and stacking interactions between nucleobases A and T and their base pairs in B-DNA have been studied by using density functional theory that includes dispersion interaction. The effect of the sugar-phosphate backbone on these interactions has also been investigated. A comparison of the interaction energy values for the Watson-Crick base pairs of A-T, Ad-Th and dMAP-dTMP reveals that both the sugar and phosphate moieties have only a marginal influence on the hydrogen bond interactions between A and T. A comparison of the interaction energy values for three different conformations of two stacked base pairs of A-T, Ad-Th and dAMP-dTMP shows that for a given conformation, the addition of the sugar moiety as well as the phosphate group does not influence the stacking interaction in a significant manner. The role of the sugar-phosphate backbone in the formation of the helical structure of B- DNA was also investigated. It is shown that the base pairs themselves have an inherent tendency to form the double helical structure and the backbone does not significantly influence the helix formation.