Energies of interactions between purine and pyrimidine bases in B- and Z-DNA.

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Abstract

The results of ab initio SCF linear combination of AO (LCAO) calcns. on the dimers on the dimers of the nucleotide bases for all possible 16 stacked configurations in B-DNA geometry, on 8 stacked conformations in Z-DNA geometry and on the Watson-Crick-type pairs in both DNA configurations are reported. In addn. to the SCF interaction energy in the supermol. approach, the contribution of the dispersion energy have been computed using London's formula with empirical parameters. In the case of the Watson-Crick-type pairs corrections for the basis-set superposition error are reported, which seem to be negligible for the stacked configuration as a calcn. on the adenine dimer shows. The results for the Watson-Crick-type pairs are in good agreement with exptl. values and with theor. ones, obtained by other methods. The stacking energies are mostly attractive but show no significant stabilization of special sequences for B- or Z-DNA. Four dimers are recalcd. with the Clementi minimal basis which leads to no considerable qual. changes in the results. As a better approach to the situation in real DNA, a qual. approxn. the charge transfer from the sugar phosphate group to the bases was taken into account. Qual., this charge transfer destablizes the pairs to some extent, namely it leads in the approxn. to a small repulsion between the stacked bases and lowers the attraction in the Watson-Crick base pairs to some extent.