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Author

Göran Wallin

Title

A study of DNA base dimers using quantum mechanical *ab initio* methods

Abstract

Ab initio quantum chemical calculations have been performed on DNA nucleobases adenine, guanine, cytosine and thymine, together with stacked dimers of guanine and cytosine to determine the effect of destacking upon rotation about the helical axis. The predicted geometries and orbital energies of the single bases were seen to correspond well with respect to experimental photoelectron spectra and averaged high resolution X-ray crystallographic structures. The potential energy along the helical rotation of the dimers showed qualitative agreement with observed B-DNA structures, where the totally stacked geometries corresponded to energetically unfavourable conformations in every studied case, with associated energy lowerings upon destacking in the order of 100-200 meV per dimer. Disagreements with the predicted dipole-dipole potential energies suggest that these lowerings may be mainly quantum mechanical in nature, and consequently caused by electron correlation and mechanisms similar to the *pseudo Jahn-Teller* effect.

Keywords

Base stacking, π-π interaction, *ab initio*, MP2, DNA

Supervisors

Prof. Leif Karlsson
Dept. of Physics, Uppsala University

Scientific reviewer

Prof. Sten Lunell
Dept. of Quantum Chemistry, Uppsala University

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Biology Education Centre Biomedical Center Husargatan 3 Uppsala
Box 592 S-75124 Uppsala Tel +46 (0)18 4710000 Fax +46 (0)18 555217