Some new results in the quantum mechanical investigation of DNA.   Ladik, J.; Otto, P.; Foerner, W..

Abstract

As a 1st step in testing the possibility of correlation calcns. of extended systems by using localized orbitals, localization of the canonical Hartree-Fock orbitals of the 4 nucleotide bases was performed. The results show an excellent localization of the occupied orbitals and a rather good one for the virtuals (both for the σ- and π-orbitals). Interaction energy calcns. of the stacked nucleotide bases show a few kilocalories/mol repulsion at the Hartree-Fock level, but they become attractive (again a few kilocalories/mol) if dispersion energy computed with the aid of London's formula is added. The internal charge transfer of .apprx.0.2 electrons from sugar to the nucleotide base electrons from sugar to the nucleotide base found in large-scale ab initio homopolynucleotide calcns. raises the question of whether there are free charge carriers in DNA B. Though in the Hartree-Fock level the answer is neg., one cannot rule out this possibility if, by using a high-quality basis set, correlated band structures (with an improved version of the electronic polaron mode) will be computed. Interaction energy calcns. between a polyglycine chain in different conformation and polynucleotide chains show a few kilocalories/mol attraction per base and glycine unit and a very small (a fraction of a kilocalorie/mol) addnl. attraction due to the dispersion correction.