E2-03 The electronic structure and properties of DNA bases and base-pairs: a semiempirical quantum mechanical study

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The investigation of the electronic structure of fragments of biologically important molecules such as nucleic acids and proteins etc. is the first step towards understanding the molecular background of biological processes. The aim of this work is to determine the specific structural features and electronic properties of DNA bases and base pairs.

The electronic structure and hydrogen bonding interactions of DNA were studied using semi-empirical quantum mechanical methods. The results of semi-empirical AM1 (Austin Model 1), PM3 (Parametric Method 3) and MNDO (Modified Neglect of Diatomic overlap) calculations on the isolated DNA bases adenine (A), guanine (G), cytosine (C), thymine (T) and A-T and G-C base pairs are presented and discussed. The similarities and differences in the electronic structure of DNA bases are discussed using the calculated electronic properties such as ionization energy, dipole moment and total net charges of atoms. The amino group nonplanarity is more pronounced for guanine and adenine than for cytosine. Thymine molecule was predicted to have a planar structure. The optimized bond angles and bond lengths of all DNA bases are in good agreement with experimental values.

The stability of the base-pairs was compared with their corresponding individual bases using the hydrogen bond formation energy. Results obtained for hydrogen-bonding distances with PM3 are very close to X-ray crystal structures than with AM1 method. The PM3 calculations on the G-C and A-T base-pairs optimized structure showed substantial deviation from coplanarity.

Financial assistance by NARESA (Research grant RG/97/C/01) is acknowledged.