Charge Transfer in DNA

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The complete set of charge transfer parameters either between neighboring bases or between successive base pairs in DNA, considering all possible combinations between them, is presented for both electrons and holes [1]. These quantities can be used in theoretical models of electron or hole transfer along the DNA double helix, as they provide the necessary parameters for a phenomenological description based on the pi molecular overlap.

Relative reaction rates for hole transfer between G radical cations and GGG triplets in DNA, through different bridges of varying length, are numerically calculated and the obtained results are compared with corresponding experimental observations [2,3]. Hole donors and acceptors are separated either by (T-A)_n bridges or by N repeated barriers consisting of (T-A,T-A) double base-pairs which are connected through single G-C base-pairs. In the former case, hole transfer rates show a strong exponential decrease with the length of the bridge for short bridges, while a switching to weak distance dependence has been observed for longer bridges. In the latter case, a power law seems to better describe the distance dependence of charge transfer rates. All these experimental observations are qualitatively reproduced by our simulations without any adjustable parameter [4]. Physical insights for the mechanism providing the switching behavior in the case of (T-A)_n bridges are presented through an analysis of the eigenfuctions of the system.

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