

HOLE TRANSFER CONFORMATIONAL DEPENDENCE IN MODELED DNA-PROTEIN COMPLEXES

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ABSTRACT

DNA can be oxidized by several agents leading to mutagenic lesions. These lesions can be produced far away from initial oxidized point because of radical cation migration through DNA. Transferring the positive charge to a binding protein or peptide will be explored. Thus, conformational study of dependence of Hole Transfer (HT) reactions in Guanine-Tryptophan (G-Trp) and Adenine-Tryptophan (A-Trp) complexes is considered. Charge transfer rate will be evaluated from electronic coupling calculations of different G-Trp and A-Trp conformations. Starting from stacked and T-shaped structures both translational and rotational freedom degrees movements are tested. It was found that HT rate is extremely dependent of the mutual position of the nucleobases and amino acids. Although stacked complexes are widely believed to have stronger couplings, a perfect stack between the aromatic rings of the system produces surprisingly weak couplings. However, the strongest coupling is obtained when only one of the two rings of the molecules is stacked. T-shaped conformations, in general, present lower HT rates than stacked structures. Even though, some T-shaped conformations have electronic couplings strong enough to ensure HT reactions.