

Photochemistry of DNA bases and base clusters

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The photochemistry of large molecules may be due to inherent properties of the light-absorbing chromophores, but can also be dominated by intermolecular interactions. The latter play a very important role in biological systems, where well defined macromolecular structure determines molecular properties and function.

We investigate the photochemistry of DNA building blocks in vacuo and reproduce the relevant intermolecular interactions of base pairing, base stacking and solvation in small molecular clusters. The combination of gas-phase spectroscopy and high-level theory allow a detailed description of excited state processes and we present examples for intra- and intermolecular reaction and relaxation pathways. From an evolutionary point of view, we expect that all DNA constituents must be highly resistant to photochemical damage, but we show that photostability is sensitively connected to tautomeric structure and intermolecular conformation.