The Photochemistry of Nucleobases from a Multiconfigurational Quantum Methods Point of View

Antonio Carlos Borin

Departamento de Química Fundamental, Instituto de Química, Universidade de São Paulo
NAP-PhotoTech, The USP Consortium for Photochemical Technology
Avenida Professor Lineu Prestes, 748, São Paulo, SP, CEP 05508-000, Brasil

The study of the photochemical mechanisms of nucleobases forming the DNA and RNA is a key step to better understanding the natural mechanisms to prevent the photodamage caused by the absorption of UV radiation.

In the case of modified nucleobases – natural or not – on which nitrogen or sulfur atoms replace some carbon atoms, the mechanisms observed are very different from those reported for their canonical counterparts. Due to that, many modified compounds are employed in phototherapeutic activities and in technological processes. By comparing the mechanisms involved in the photochemistry of the modified nucleobases against those of their canonical counterparts is a good way to find out molecular patterns that can be useful for the design of new drugs and technological compounds.

In this work, we will present a brief review about the photochemistry of modified and canonical nucleobases, aiming to establish a pattern to explain the observed differences, employing, basically, ab initio multiconfigurational methods. They are necessary for describing the electronic nature of the singlet and triplet excited electronic states and the nonadiabatic pathways.