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Light and Nucleobases: A Healthy Relationship

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Abstract: We are used to thinking that light, especially in the ultraviolet region, is not good for us because it has a destructive influence on DNA and RNA; UV radiation, for instance, is the main agent for DNA mutagenic effects. Nonetheless, they (nucleobases and radiation) co-exist since ancient times, even without the protective ozone. So, we may wonder: how did the nucleobases survive under such extreme conditions? Is it due to a kind of natural protection mechanism? Answering this question is important, because if we understand the photochemical mechanisms behind this longstanding relationship, we can learn how to minimize the damage and maximize the profit. The canonical nucleobases are photostable due to extremely efficient nonradiative photochemical pathways, which makes them very low fluorescent species. Which are the photochemical pathways responsible for ultrashort lifetimes of the canonical nucleobases?

On the other hand, a good way for studying DNA/RNA structure and dynamics is to use fluorescence spectroscopy; but, if the canonical nucleobases are not fluorescent, how is it possible to employ fluorescence spectroscopy? The answer is on fluorescent natural and non-natural modified nucleobases, especially those that are isomorphic to the canonical species, which besides fluorescent probes can be employed to artificially expand the genetic code. Which are the photochemical mechanics and nature of their excited states?

In this work, we will present an overview of the photochemistry of modified and canonical nucleobases, based on results derived with the aid of high level, state of the art ab initio multiconfigurational methods. By exploring similarities and differences, we can better understand the fundamental aspect behind the interaction of light and nucleobases and, in some sense, make proposals for how to obtain fluorescent species.

Key-words: Canonical nucleobases, modified nucleobases, photochemical mechanisms, luminescence, multiconfigurational ab initio methods

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