A theoretical study on the OH/H radical addition to DNA/RNA pyrimidines and the photochemistry of the adducts

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Cellular DNA is constantly exposed to reactive species that can alter the natural structure of the DNA/RNA nucleobases.[1] It has been demonstrated that an unbalanced oxidative stress can cause DNA-protein crosslinking and/or DNA/RNA strand breaking, producing mutations in the genetic material. These modifications may ultimately lead to cell death or even serious diseases like cancer or neurodegeneration, among others.[2] Understanding the complex mechanisms behind this important processes at the molecular level requires the contribution of both experimental and theoretical approaches.

In the present communication, we will discuss on recent findings obtained in the theoretical study of the OH/H radical addition to the C5=C6 double bond of DNA/RNA pyrimidines.[3,4] The ground-state reactivity between the free radicals and the nucleobases, as well as the absorption properties and photochemistry of the formed adducts have been determined by means of the CASPT2//CASSCF protocol. The findings help to interpret the experimental observations recorded during the last decades and shed light into the molecular mechanisms of the DNA/RNA damage.

References

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