Study of Photorelaxation Pathways in 7H and 9H Tautomers of 2,6-Diaminopurine

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Understanding the ultrafast relaxation mechanisms of photoexcited nucleobase analogs is crucial for elucidating their photostability and potential biological implications. In this study, we employ nonadiabatic molecular dynamics simulations with surface hopping to investigate the ultrafast relaxation mechanisms of 2,6-diaminopurine in both its 7H and 9H tautomeric forms. Simulations are performed in vacuum and aqueous solution (implicit water clusters) using DFT/TDDFT electronic structure. Our results highlight the influence of solvation and on the excited-state dynamics and the role of conical intersections in system relaxation back to the ground state. This study provides deeper insights into the photophysics/photochemistry of purine derivatives and their implications for photostability in biological and biomimetic systems.