SINGLE-CONFORMATION SPECTROSCOPY AND DYNAMICS ON MULTIPLE POTENTIAL ENERGY SURFACES: FLEXIBLE NITROGEN-HETEROCYCLE CHROMOPHORES AND COMPLEXES IN AEROSOLS

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The interplay between chemical functionality and structure is a key factor in the photophysics and photochemistry of complex, flexible molecules, often giving rise to multiple potential energy surfaces. Adequate description of this relationship to understand the outcomes and properties of polyatomic molecules is made even more difficult as the number of isomers and conformations increase substantially with the size of the system. The inclusion of water-mediated interactions is often needed due to dramatic effects on the conformational preferences and photophysics. Therefore, the synergy between spectroscopy and chemical dynamics methods is required to obtain a molecular-level view of such complex chemical systems. To address these opportunities, we will illustrate our efforts to investigate the intermolecular interactions of molecular complexes using single-conformation spectroscopy and dynamics techniques to probe the photo-initiated outcomes on multiple potential energy surfaces. Thus, the photophysical, photochemical and structural details of the target conformational isomers and complexes enable multifaceted comparisons to several theoretical predictions.