Investigating Excited State Pathways of Schiff Base Targets Using Raman Spectroscopy

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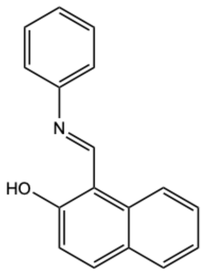
Proton transfer (PT), the movement of protons from one molecule to another, is present in many chemical and biological processes. Photoacids release protons upon irradiation during excited state proton transfer (ESPT), making them a useful tool for researching time-resolved PT. Throughout the summer, I worked on two projects centralized around identifying and characterizing photoacids.

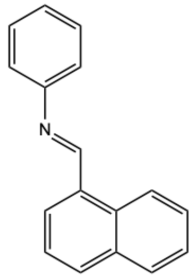
The beginning of the summer focused on a training project about the classification of 2-naphthol, a well-studied molecule in literature, as a photoacid. I received an introduction to the UV absorption and emission instruments, as well as the time-correlated single photon counting emission spectrometer (TCSPC). 2-naphthol is a simple photoacid with only one pathway in the excited state, which ensured accuracy in the data I was collecting. Collectively, this project visualized the process of ESPT from both a thermodynamic and kinetic perspective.

The second project, which I will continue throughout the upcoming fall and spring, revolves around Schiff base targets (compounds 1-4). As more structurally complex molecules enter the excited state, different pathways become more prevalent. In the case of Schiff base targets, they have the potential to travel through different pathways than ESPT, such as photoisomerization. Raman spectroscopy uses vibrational motions in order to characterize molecules' structures. I am adapting this approach by studying the compounds in the excited state. By shining light on a sample within the Raman spectrometer, I am analyzing how the structure of the targets changes in real-time. Depending on the change in structure, the pathways gone through by the compounds can be concluded.

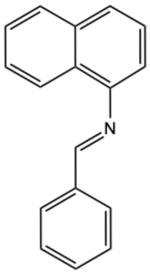
compound 1:



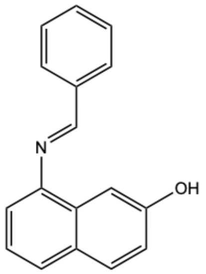
compound 2:



compound 3:



compound 4:



So far, the Raman spectra have been taken of each molecule in the ground state. The samples were then shined with a 254 nm wavelength light, which displayed the excited state spectrum on the Raman. However, after analyzing samples which do not enter the excited state, they 'changed form' on the Raman after light excitation as well. It was theorized that the 259 nm light source excites certain molecules in the air that overshadow the excited Schiff base targets' structural changes. Therefore, a light source needs to be found that possesses a wavelength that will solely excite the targets.

In the future, I aim to find light sources that will not interfere with the data collection of the Schiff base targets in the excited state. After that is complete, I will continue to characterize the structural differences of the compounds in their respective ground and excited states. Finally, I will extend my library of Schiff base targets to determine how more variations of the compound affect their excitation pathways.

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