

Changing the Excited State Proton Transfer Pathway of 8-amino-2-naphthol with Acetonitrile and Water

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Photoacids are compounds known for their increased acidity upon light excitation and their ability to undergo excited state proton transfer (ESPT). They are used in a variety of applications, ranging from biological to industrial. These applications can occur in different solvents; thus, it is important to understand how the solvent can affect the mechanisms of ESPT for photoacids.

In continuation of the work of former lab member, Gabby Vandendries, I studied the proton dynamics of 8-amino-2-naphthol (8N2OH) in both acetonitrile (CH_3CN) and water (H_2O). 8N2OH was chosen as it has two sites that can potentially undergo ESPT when excited from its cationic ground state. The two possible sites for ESPT are located at the hydroxyl and amine groups (Figure 1). The two solvents have different hydrogen bonding capabilities, specifically, acetonitrile is only a hydrogen bond acceptor while water is both a hydrogen bond acceptor and donor. These differences have the possibility to influence the mechanisms of ESPT as they can influence electron density distribution and stability of 8N2OH in the excited state.

To study the mechanisms of ESPT for 8N2OH, I used a combination of absorption and time-resolved emission spectroscopy to observe both the ground and excited states respectively. The absorption spectra of 8N2OH showed no significant difference between the two solvents, indicating that the ground state was the same for both solvents. In looking at the excited state, the steady state emission spectra of 8N2OH had significantly different features between the two solvents. This meant that different species existed in the two solvents after excitation. The decay lifetimes confirmed this and indicated different mechanisms of ESPT in water and acetonitrile. We concluded that in water, the ESPT occurred at the hydroxyl group, while ESPT occurred at the amine group in acetonitrile. In addition, we performed further chemical testing at the amine group using crown ether to better understand the proton dynamics involved.

Thus, we have shown that we can tune the mechanisms of ESPT by changing the solvent environment. Further explorations will involve observing how mixtures of solvents can affect the possible pathways for ESPT and studying 8N2OH in other classes of solvents.

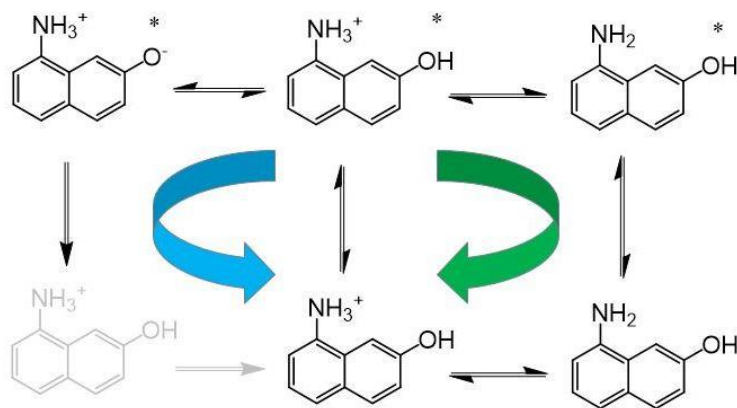


Figure 1. Possible Pathways for ESPT in 8-amino-2-naphthol

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