Proton Transfer in 3-amino-2-naphthol

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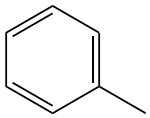
Proton transfer (PT) is an essential process in photosynthesis and artificial photosynthesis[1]. In order to optimize these systems, it is necessary to understand PT and be able to model it. In the Takematsu lab, aminonaphthols are used to model PT. Aminonaphthols are photoacids, which means that they become significantly more acidic upon excitation. Therefore, it is possible to use light to trigger PT and to access different protonation states.

For this project, the molecule of interest was on 3-amino-2-naphthol (3N2OH). This molecule has a similar structure as 2-naphthol, a well characterized[2-3] photoacid. In 3N2OH there is an added amine (NH_2/NH_3^+) group on the carbon adjacent to the alcohol (OH) group. This allows us to study how the proximity of the amine functional group affects PT. PT can occur either between the two functional groups as intramolecular PT or between each functional group and the solvent as intermolecular PT. In the ground state, there are three possible protonation states, the cation, neutral, and anion (Figure 1). The protonation state of the molecule depends on the pH of the system and the pK_a of each functional group. In the ground state, the pK_a of the NH_2 group is 3.9 ± 0.1 and the pK_a of the OH group is 9.1 ± 0.1.



* of the OH group. It acts as a switch, dictating whether or not 3N2OH is photoacidic.

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References:

1. Mora, S. J.; Odella, E.; Moore, G. F.; Gust, D.; Moore, T. A.; Moore, A. L., Proton-Coupled Electron Transfer in Artificial Photosynthetic Systems. *Accounts of Chemical Research* **2018**.

2. Lee, J.; Griffin, R. D.; Robinson, G. W., 2-Naphthol: a simple example of proton transfer effected by water structure. *J. Chem. Phys.* **1985,** *82* (11), 4920-5.

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