Nantes Université

Proposition de Stage Master CMT

Stage de M1 ☒ et/ou Stage de M2 ☒

Titre du stage : Modeling the Excited State Reactivity and Photophysics of 3-hydroxychromone

Equipe d'accueil : ModES team (CEISAM lab)

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Description du stage proposé :

Excited state reactivity plays a fundamental role in photochemistry. Gaining a deeper understanding of how molecules behave in their excited states is critical for rationalizing complex reaction mechanisms and controlling (photo)chemical reactions. 3-hydroxychromone (3-HC), has been extensively studied [1,2,3] for its ability to exhibit excited state intramolecular proton transfer (ESIPT) upon excitation to the S_1 or S_2 electronic state (see *Figure 1*). Previous experimental work [1], using time-resolved UV-vis absorption spectroscopy, detected two time constants associated with the proton transfer reaction in the excited state: one on the femtosecond timescale and the other on a longer timescale. Although the photodynamics of the system have also been investigated by means of theoretical-computational approaches [2,3], the origin of the double timescale associated with the proton transfer reaction has only been hypothesised.

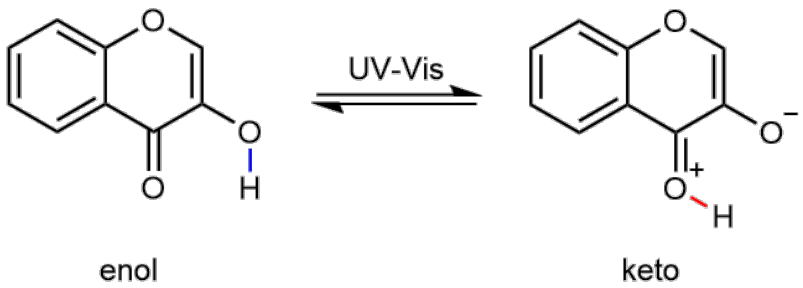

Figure 1. Excited state intramolecular proton transfer (ESIPT) in the 3-HC molecule upon excitation to the S_1 or S_2 electronic states.

The objective of this study is to explore the excited-state reactivity of the 3-HC system in the gas phase, focusing on the ESIPT process as well as possible competing pathways, such as the out-of-plane torsion of the hydrogen atom, which may slow down a fraction of the population undergoing proton transfer (see *Figure 2*). Using advanced computational methods, including full- and reduced-dimensionality [4] surface-hopping dynamics, we aim to identify the relevant nuclear coordinates involved in the ESIPT reaction and the possible competing pathways.

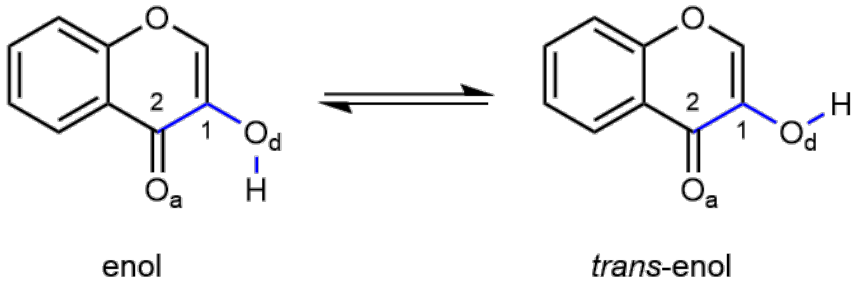

Figure 2. Enol to *trans*-enol conformational equilibrium of 3-HC.

Bibliography

1. Chevalier, K. et al. *J. Phys. Chem. A* **2013**, 117, 11233
2. Nag, P. et al. *J. Chem. Phys.* **2021**, 155, 094301
3. Perveaux, A. et al. *Phys. Chem. Chem. Phys.*, **2017**,19, 6579
4. Delmas, V. et al. *J. Chem. Theory Comput.*, **2025**, 21, 13, 6611

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