

## A three-state model for Photo-Fries rearrangement

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Photo-Fries rearrangement (PFR) is a photochemical conversion of aryl esters to *ortho*- and *para*-hydroxyphenones. This reaction is a key step in the synthesis of a large number of compounds and plays an important role in designing of functional polymers and for photodegradation of drugs and agrochemicals. In particular, photodegradation of aromatic carbamates, widely used as pesticides, can be governed by photo-Fries rearrangements. Although there are a large number of experimental studies on PFR, the last theoretical work is from 1992 and some points of this reaction are still under debate. Given the knowledge gap between theory and the most recent experimental works, our aim has been to provide a comprehensive picture of PFR, based on high-level multiconfigurational theoretical methods. In this seminar, I will present the three-state model which we propose to explain the PFR. It provides a comprehensive mechanistic picture of all steps of the reaction, from the photoabsorption to the final tautomerization. I will also show the effect of substituents and our efforts to understand the role of solvent in this reaction.