

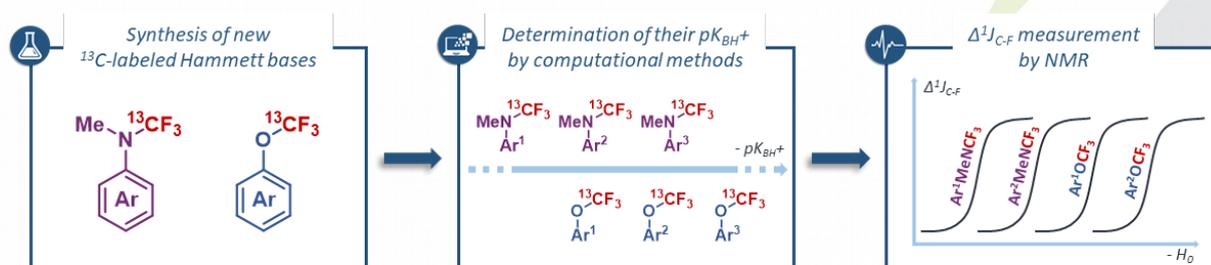
PhD position IC2MP –POITIERS

H-Scale: determination of the Hammett acidity function of emerging protic media by combining NMR and DFT studies

Starting date: October 2021

Applications are invited for a PhD Fellow position at the Institute of Chemistry of Poitiers (IC2MP UMR CNRS 7285) / University of Poitiers to work on a project for the development of a new method to characterize the acidity of emerging protic media in organic synthesis.

Last years have witnessed the emergence of new synthetic strategies relying on the acidic properties of anhydrous protic media. Unlike aqueous acids whose acidity can easily be determined using the pH scale, the quantification of the acidic character (acidity function) of these new media remains highly challenging. This project, merging organic synthesis, NMR analysis and DFT calculations, aims at developing a new method for determining the Hammett acidity function of acidic and superacidic media. More specifically, this method will rely on $^1J_{C-F}$ measurements using ^{13}C -labeled $N-CF_3$ -anilines and $O-CF_3$ -phenols. The first goal of this project will be the synthesis of a large library of anilines and phenols substituted by a CF_3 group. In a second time, their basicity will be assessed by DFT calculations. These new NMR probes will then be applied for determining the acidity of protic media of interest in the field of organic chemistry.



Application to the acidity evaluation of new protic media (Hammett acidity function H_0)

Applicants must have completed a master degree in organic synthesis or physical organic chemistry, and have acquired an experience in organic synthesis. The candidate should have the drive and enthusiasm to see the project from fundamental research to design, regarding both theoretical and experimental aspects in the project. Knowledge in molecular modeling is an asset, but doctoral degree training in computational methods is also available locally. S/he should be able to work independently and as a member of both teams. The optimal candidate will be inquisitive, will enjoy problem solving and developing novel technologies with personal creativity and innovation. Interested and highly motivated applicant should forward a **cover letter** stating why the applicant is interested in this position, a **complete CV** and at least **one recommendation letter**.

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