

Research Grants for PhD students from the China Scholarship Council

Information Form (please read the guidelines carefully on the website www-csc.utt.fr)

Supervisor's name : JUBAULT Given names : PHILIPPE

Status (prof., assistant prof., ...) : Professor of Chemistry

Laboratory : CARMeN Institute - UMR 6064 Website address : <http://www.lab-cobra.fr>

Institution : Institut National des Sciences Appliquées - Rouen Website address : <https://www.insa-rouen.fr/recherche/laboratoires/carmen>

Scientific competence of the supervisor:

Our research group is interested in the development of new synthetic methodologies for strategic C-C bond formations using energy-efficient technologies. In this field, our efforts are particularly targeted towards the mechanistic understanding of the chemical reactions we develop.

Two major publications in the field proposed for the PhD :

1. Ammer, J.; Nolte, C.; Mayr, H. Free Energy Relationships for Reactions of Substituted Benzhydrylium Ions: From Enthalpy over Entropy to Diffusion Control. J. Am. Chem. Soc. 2012, 134 (33), 13902–13911.
2. Mayr, H.; Bug, T.; Gotta, M. F.; Hering, N.; Irrgang, B.; Janker, B.; Kempf, B.; Loos, R.; Ofial, A. R.; Remennikov, G.; Schimmel, H. Reference Scales for the Characterization of Cationic Electrophiles and Neutral

Website address of the personal page : <https://www.insa-rouen.fr/recherche>

Supervisor's email : philippe.jubault@insa-rouen.fr

Description of the research work proposed for a PhD

Topic # (see list) : II-13

Title : Kinetic Investigations of Transient Carbocations

Subject :

Ubiquitous intermediates in many transformations taught from the very first years of organic chemistry, carbocations remain highly studied species, particularly due to their ability to promote spectacular skeletal rearrangements. Beyond the elementary reaction steps of SN1 and E1, carbocations participate in numerous thermodynamically-controlled rearrangements, such as Pinacol and Wagner-Meerwein rearrangements. Despite their predominance in many reaction mechanisms, their reactivity has been insufficiently studied from a kinetic perspective. More specifically, existing studies have primarily focused on the addition rates of different nucleophiles to stable and well-defined carbocations, leading to Mayr's valuable electrophilicity scale. This research program will be dedicated to the reactivity of non-stabilized carbocations, with particular emphasis on the rates of nucleophilic additions to these species relative to their rearrangement rates. Ultimately, this project aims to expand Mayr's database and provide the scientific community with a reliable tool for studying cationic reactions. To support this research program we are looking for an outstanding and highly motivated candidate to pursue his PhD within our group.

Keywords :

carbocations ; kinetic study

Expected collaborations :

Background required from the applicant :

A Master degree in Organic Chemistry, good knowledge of the analytical methods (NMR, MS...)

Existence of a PDF file detailing the proposal ("yes" or "no") :

(see guidelines on the website www-csc.utt.fr)