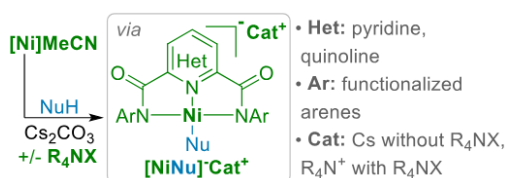


POST-DOCTORAL POSITION (13 months from February 2025)
Mass spectrometry characterization of reaction mechanisms involving nickel catalyzers

Context, project description and objectives

Potent catalysts and catalytic systems are currently considered as strategic tools for chemists in quest of sustainable chemistry, with the aim of increasing molecular complexity in a selective (atom-economy) and efficient manner (time and energy economy). In this project, we propose to investigate, by mass spectrometry, chemical reactions catalyzed by nickel complexes (Scheme 1), which have been proven to yield efficient cyanoalkylation of isatin derivatives.



Scheme 1: Nickel ate-complexes as ion pairs in catalysis

The post-doctoral will study the reaction mechanism through the structural characterization of short-lived and polar organometallic complexes and intermediates. Depending on the studied complexes/intermediates, electrospray (ESI), atmospheric pressure photoionization (APPI) or laser desorption ionization (LDI) techniques will be combined with ion mobility spectrometry and high-resolution mass spectrometry (TIMS-FTICR 18 T, TIMS-Q-TOF or TWIMS-Q-TOF). *In situ* analysis of the reactions will be carried out, either by direct introduction (infusion, flow injection analysis) or using a microreactor, depending on the reaction kinetic. Structural information will be obtained by tandem mass spectrometry and collision cross sections (CCS) determination that will be compared to calculated values from DFT investigation.

Activities: Optimization of ionization conditions (ESI, APPI and LDI) for the different nickel complexes and implementing the microreactor approach, performing IMS-HRMS(/MS) experiments using the appropriate ionization technique and data processing. Bibliography, presentation and publication of results.

Candidate profile and skills: - PhD in mass spectrometry with good general technical skills in HRMS, MS/MS and in ESI, eventually in APPI and LDI.

- Skills in organization and in communication to work within a team, independence, enthusiasm, good knowledge of written English

Selection process and deadlines: The applicant should provide a CV, a cover letter, recommendation letters or contact of reference persons to Pr Carlos Afonso (carlos.afonso@univ-rouen.fr) / Dr Corinne Loutelier-Bourhis (corinne.loutelier@univ-rouen.fr) and Dr Marie Hubert-Roux (marie.hubert@univ-rouen.fr). After preselection, the preselected candidates will be invited for an interview.

Application must be sent before December 15th 2024.

Post-doctoral duration: 13 months, financed by the Agence Nationale de la Recherche (ANR) (Gross salary : 2800-2900€/month)

To start: from february 2025

Host laboratory: COBRA UMR CNRS 6014 laboratory (University of Rouen Normandie).

References:

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- [2] Lespes, N.; Pair, E.; Maganga, C.; Bretier, M.; Tognetti, V.; Joubert, L.; Levacher, V.; Hubert-Roux, M.; Afonso, C.; Loutelier-Bourhis, C.; Brière, J.-F. Chem. Eur. J. 2018, 24, 4086.
- [3] Lebrêne, A.; Martzel, T.; Gouriou, L.; Sanselme, M.; Levacher, V.; Oudeyer, S.; Afonso, C.; Loutelier-Bourhis, C.; Brière, J. F. J. Org. Chem. 2021, 86, 8600.
- [4] Ramírez-Pradilla, J. S.; Blanco-Tirado, C.; Hubert-Roux, M.; Giusti, P.; Afonso, C.; Combariza, M. Y. Energy & Fuels 2021, 35, 14542.