Secteur des Sciences et Technologies

Invitation à la soutenance publique de thèse de

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Master en Sciences chimiques à finalité approfondie

Pour l'obtention du grade de Docteur en sciences

« NMR Spectroscopy as a tool to study homogeneous copper (I) catalysed reactions »

qui se déroulera
le vendredi 13 mars 2020 à 16h
Auditoire SUD 09
Place Croix du Sud
1348 Louvain-la-Neuve

Jury members :

Prof. Tom Leyssens (UCLouvain), supervisor
Prof. Olivier Riant (UCLouvain), supervisor
Prof. Yann Garcia (UCLouvain), chairperson
Dr. Gabriella Barozzino Consiglio (UCLouvain), secretary
Prof. Michel Luhmer (ULB, Belgium)
Dr. Christian Kleeberg (TU Braunschweig, Germany)
Prof. Daniel Peeters (UCLouvain)

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This thesis contributes to the general aim of pushing the boundaries of scientific knowledge a little further in the field of copper chemistry.

Here is depicted the use of Nuclear Magnetic Resonance spectroscopy, more specifically 1D 1H and 2D 1H Diffusion-Ordered Spectroscopy, as a tool to elucidate the solution-state nature of copper (I) complexes and to investigate their implication in the reaction mechanism of the catalysed borylation of unsaturated carbon-carbon bonds.

The first part is focused on the extrapolation of the molecular sizes of the complexes from their translational self-diffusion in solution, using two different methods (Morris and Williard), both based on the experimental Stokes-Einstein equation describing the Brownian motion of particles in solution and its relationship with the size of these particles.

The second part is based on the understanding of the copper (I)-mediated borylation of unsaturated carbon-carbon bonds and of the characterisation of the transient copper (I) complex intermediates of the reaction mechanism. Through a novel and simple *out-of-the-glovebox in situ* NMR investigation method, the existence of literature-reported structures is confirmed and the identification and characterisation of unprecedented copper (I) alkyl, benzyl, alkenyl and allyl complex intermediates are described.

The myriad of reactions and various copper (I) complexes studied in this thesis show the high versatility of this *in situ* method, and it paves the way for the investigation of many other reaction mechanisms.