

Title of the thesis	NMR characterization and antimicrobial activity of mechanically synthesised organometallic complexes
Acronym	NMR-MECA-DRUG
Reference number	008

Hosting institution	Employer
Université de Lille Website: https://www.univ-lille.fr/home/	CNRS Website: http://www.cnrs.fr/en
Hosting research unit 1	Hosting research unit 2
Name: Unité de Catalyse et de Chimie du Solide Acronym: UCCS Identification number: UMR 8181 Address: Université de Lille Bâtiment C3 59655 Villeneuve d'Ascq Cedex Website: http://uccs.univ-lille1.fr/index.php/en/	Name: Lille Inflammation Research International Center Acronym: LIRIC Identification number: U995 Address: Faculté de Médecine – Pôle recherche, Place Verdun, 59045 Lille Cedex Website: http://lille-inflammation-research.org/fr/
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Thesis information	
Keywords	solid-state NMR; antimicrobial activity
Abstract	<p>In order to develop greener manufacturing processes, there is a need to reduce or even eliminate the use of solvents, which can entail pollution, risks for human health and the exploitation of fossil resources. Mechanochemistry is a promising route to achieve this goal. However, there is currently limited insight into the mechanisms of these solid-state reactions. This PhD project will aim at demonstrating the potential of solid-state Nuclear Magnetic Resonance (SSNMR) to examine the changes in the atomic-level structure during mechanosynthesis (even for amorphous phases) and the evolution in real time of chemical reactions. The magic-angle spinning (MAS) used in SSNMR will permit to mimic the conditions of mechanosynthesis and to carry out in situ NMR measurement, allowing the observation of fleeting intermediates. These studies will be performed on the NMR facility of the University of Lille (ULille), which is a leading one at international level (with high-field NMR magnets: 800 and 900 MHz, as well as 1.2 GHz from 2021, with several probes).</p> <p>The targeted mechanosynthesis is that of organometallic complexes that exhibit antimicrobial (AM) activities. This PhD project will further assess these activities using biological tests and will investigate their mode of action against bacterial strains,</p>

	<p>notably Gram-positive <i>S. aureus</i> and <i>S. epidermidis</i> bacteria, including resistant ones, which are the most common pathogens causing infections of implants (catheters and artificial prosthetics). Besides the complexes, this project will investigate the AM activity of metallate intermediates, that are so far unknown.</p> <p>The goal of this project is to develop new AM agents and help address the prevalence of AM resistance, which is currently one of the greatest challenge to public health. In summary, the PhD thesis subject is the "study of mechanosynthesis mechanisms for organometallic complexes with anti-microbial activity". It is an ambitious multidisciplinary project, combining SSNMR spectroscopy, mechanochemistry, organometallic chemistry and bacteriology.</p> <p>The involved academic laboratories are the Unité de Catalyse et de Chimie du Solide (UCCS) UMR 8181 ULille-CNRS, the Lille Inflammation Research International Center (LIRIC) U 995 ULille-INSERM and the Department of Chemistry at Ghent University (UGent). The PhD student will be supervised by professor Olivier Lafon (UCCS) for SSNMR, Dr. Christel Neut (LIRIC) for biological tests and professor Catherine Cazin (UGent) for mechanochemistry. The PhD student will spend 29 months at ULille and 6 months at UGent, and the PhD can be realized as a cotutelle between both universities.</p> <p>The student will also perform a one-month secondment in Bruker company in Germany, which will reinforce his employability and will permit him to test very fast MAS.</p> <p>The student will attend summer school on SSNMR and will present the results of the project in national and international congress (OMCOS 2021, ENC 2022, ISMAR 2023). Final competences and employability: after completion of the project, the candidate will have gained a unique expertise in analytical, biological and synthetic chemistry; and a unique international multidisciplinary experience. (S)he will have a highly attractive profile of interest to most industry segments as well as academic research units.</p>
Expected profile of the candidate	<p>The candidate must be dynamic, committed, with strong adaptability and communication skills, and holding (or will be holding) a M.Sc. in Chemistry or Pharmacology. Experience in NMR spectroscopy, chemical synthesis and/or biological tests is a plus.</p>
Application procedure	<p>The application procedure is detailed on the European programme PEARL website www.pearl-phd-lille.eu. The funding is managed by the I-SITE ULNE foundation which is a partnership foundation between the University of Lille, Engineering schools, research organisms, the Institut Pasteur de Lille and the University hospital.</p> <p>The application file will have to be submitted before April 15, 2020 (10h Paris Time) and emailed to the following address : international@isite-ulne.fr.</p>
Net salary and Lump Sum	<p>A net salary of about €1,600 + €530 per month to cover mobility, travel and family costs.</p>