

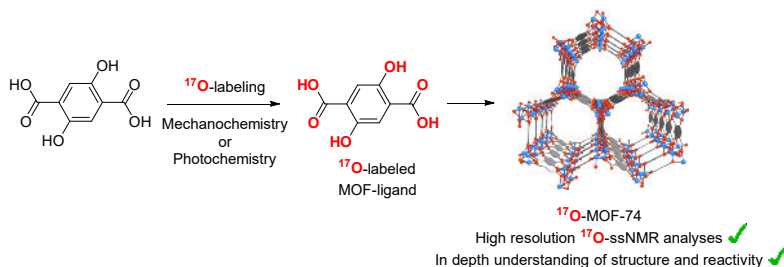
## Master 2 / Engineer internship (6 months): Advancing carbon capture research thanks to <sup>17</sup>O-labeling of MOFs

### Project description

With the increase in CO<sub>2</sub> concentration in the atmosphere, there is an urgent need to reduce our emissions and develop means to capture this gas in an efficient and durable way. A wide variety of materials have been tested and studied for this purpose, including porous compounds like zeolites and MOFs (Metal-Organic Frameworks). However, to help understand and further optimize the properties of these materials, it appears necessary to analyze their structure in more depth, including at the atomic scale. The general purpose of this project is to participate to the development of advanced NMR-based techniques for studying the structure of MOFs currently being developed for CO<sub>2</sub> capture. The focus will be set on helping analyze in depth the local environment of the oxygen atoms present in the ligands which make up these MOFs, using <sup>17</sup>O NMR. Indeed, the role of the ligands is central in defining the overall structure of the material, but also, in some cases, the reactivity which can take place within the pores, upon incorporation of small molecules.

To date, oxygen-17 NMR has only been used in a small number of cases for the investigation of MOFs, due to the very poor natural abundance of <sup>17</sup>O (only 0.04 %). Therefore, in this project, the objectives will be:

- to develop novel efficient <sup>17</sup>O-enrichment schemes of ligands which are commonly used in MOFs, by using synthetic techniques like mechanochemistry or photochemistry,<sup>1,2</sup>
- to characterize the labeled ligands by a variety of analytical techniques (to evaluate their enrichment level), including mass spectrometry and <sup>17</sup>O solid state NMR;
- to use these labeled ligands for the preparation and analyses of a selection of <sup>17</sup>O-enriched MOFs.



### Research environment

Research will be carried out at the Institut Charles Gerhardt (ICGM, UMR5253) of the University of Montpellier (<https://www.icgm.fr/>), within the MISOTOP research group (<https://www.misotoplab.org/>). The ICGM is internationally renowned for its expertise in materials science, with an excellent support for advanced studies on their synthesis and characterization. The MISOTOP group is fully equipped for <sup>17</sup>O isotopic labeling (with 7 ball-mills for mechanochemistry, and UV-lamps for photochemical reactions), and for the analysis of the enriched compounds (including by mass spectrometry and solid-state NMR).

On a daily basis, the recruited student will work under the supervision of Drs Thomas-Xavier Métro and Danielle Laurencin. He/she will also have the opportunity to interact with the team of researchers, engineers, and students involved in this study both locally (in Montpellier), and at the national level, notably with the groups of Dr F. Pourpoint in Lille and Prof C. Gervais in Paris.

### Application procedure

This project is funded by the French national research funding agency (ANR). The starting date for the internship is planned for early 2026. To apply, send a CV, motivation letter, and the names of 2 references to both Drs Thomas-Xavier Métro ([thomas-xavier.metro@umontpellier.fr](mailto:thomas-xavier.metro@umontpellier.fr)) and Danielle Laurencin ([danielle.laurencin@umontpellier.fr](mailto:danielle.laurencin@umontpellier.fr)). Candidacies will be examined until the position gets filled.

### References

- (1) Métro, T.-X.; Gervais, C.; Martinez, A.; Bonhomme, C.; Laurencin, D. Unleashing the Potential of <sup>17</sup>O NMR Spectroscopy Using Mechanochemistry. *Angew. Chem. Int. Ed.* **2017**, *56* (24), 6803–6807. <https://doi.org/10.1002/anie.201702251>.
  - (2) Doussot, A.; Bakai, M.-F.; Fouquet, E.; Hermange, P. *Ex Situ* Generation of <sup>18</sup>O<sub>2</sub> and <sup>17</sup>O<sub>2</sub> from Endoperoxides for <sup>18</sup>O-Labeling and Mechanistic Studies of Oxidations by Dioxxygen. *Org. Lett.* **2023**, *25* (25), 4661–4665. <https://doi.org/10.1021/acs.orglett.3c01487>.
- NB: Image of MOF-74 taken from reference : Xiao, T.; Liu, D. The Most Advanced Synthesis and a Wide Range of Applications of MOF-74 and Its Derivatives. *Microporous Mesoporous Mater.* **2019**, *283*, 88–103. <https://doi.org/10.1016/j.micromeso.2019.03.002>.