Developing non-precious transition metal based catalysts for hydrogenation reactions and their use in para-hydrogen induced hyperpolarization based applications

Summary

This PhD research project will focus on designing and synthesizing suitable first row transition metal complexes capable of binding H2 in reversible manner to carry out hydrogenation reactions. While doing so, the successful candidate will dwell into the world of organometallic chemistry to design, synthesize and utilize custom made ligands on the selected non-precious metal salts. These complexes would then be assessed in hydrogenation reactions to evaluate their para-hydrogen induced polarization transfer efficiency. This fully funded PhD project will offer the candidate an opportunity to learn the skills necessary to carry out air- and moisture sensitive chemistry using organometallic complexes, and secondly it will expand the application of these complexes into solution NMR to increase the signals of low concentration analytes in a mixture of interest. The overall goal of the project is to test and find the structurally simplest non-precious metal complex capable of inducing NMR signal enhancement in presence of para-hydrogen (p-H2) and suitable selection of substrates. The project addresses the following research questions: Which non-precious metal based system is suitable for redox chemistry application? Which types of ligands have an important effect of the reversible binding of H2? How different types of substrates of interest interact with these metal complexes?

Research field:	Chemistry and biotechnology
Supervisor:	Dr. Martin Jakoobi
Availability:	This position is available.
Offered by:	School of Science National Institute Of Chemical Physics And Biophysics
Application deadline:	Applications are accepted between June 01, 2025 00:00 and June 30, 2025 23:59 (Europe/Zurich)

Description

The research

While non-destructive as an analytical technique, NMR analysis of complex mixtures (petrochemical fractions, biofluids, soil samples etc.) is cumbersome due to limited sensitivity of NMR samples under thermal equilibrium conditions. However, where there is a scientific problem, there is a scientific solution to overcome this issue of NMR insensitivity. Namely, various research groups have reported more than 1000-fold sensitivity gains by employing cleverly designed experiments under para-hydrogen induced polarization (PHIP) conditions. Our colleagues at KBFI, among other research groups, have demonstrated the possibility of detecting sub-micromolar quantities of metabolically relevant analytes and even oligopeptides [1]. As the field is still developing and trying to break through the academic boundaries to become a day-to-day analytical technique, the affordability of the most studied iridium based catalytic systems in the long run needs to be addressed. First promising steps to employ non-precious metal based PHIP catalysts have been developed Fout's group [2,3], which has inspired us to investigate this angle even further.

The aim of the PhD project is to develop and synthesize non-precious transition metal complexes capable of reversibly binding H2 and carrying out hydrogenation reactions of unsaturated functional groups. The PhD candidate will explore the synthesis and effect of custom-made ligands on the metal center and how these changes will affect the possibility to carry out NMR signal enhancement using PHIP transfer. The outcome of his/her results in developing and applying simple and cheap metal complexes in PHIP signal enhancement process would allow research community to leap forward by making these complexes affordable for daily use in analytical chemistry and reaction mechanism studies.

The project is inherently interdisciplinary and will combine our expertise in several chemistry disciplines. The PhD candidate will be exposed to organic and organometallic chemistry, NMR spectroscopy, and to catalytic processes. Prior exposure to one or more of these disciplines and enthusiasm in learning the handling of organometallic compounds will be seen as a plus.

Responsibilities and (foreseen) tasks

- Getting acquainted with current state-of-the-art research in the field.
- Willingness to deeply dwell into the air and moisture sensitive chemistry of transition metal complexes.
- Being curious to learn more about NMR and the suitable scope of potential target substrates that could be detected under *p*-H_2 induced polarization transfer process.
- Preparing, storing, utilizing correctly sensitive reagents, complexes and different solvents.
- Contribute to departmental seminars and participate at scientific events.
- Develop reform proposals and suggestions for practice
- To obtain teaching experience while supervising BSc/MSc students.

Applicants should fulfil the following requirements:

- a master's degree in chemistry (preferably in organic, inorganic or homogeneous catalysis)
- hands of experience in synthesizing, purifying and characterizing compounds
- a clear interest in the topic of the position
- excellent command of English
- strong and demonstrable writing and analytical skills
- capacity to work both as an independent researcher and as part of an international team
- capacity and willingness to provide assistance in organizational tasks relevant to the project

(The following experience is beneficial:)

- enthusiasm in learning the handling of organometallic compounds will be seen as a plus
- knowledge and experience in liquid NMR
- independent nature and willingness to test one's ideas
- ability to work in collaboration with other groups and individuals of different seniority in academia

We offer:

- 4-year fully funded PhD position in one of the most internationalized research centers in Estonia at KBFI (Keemilise ja bioloogilise füüsika instituut) where the synergy between chemistry, biology and physics can lead to new frontiers in science.
- Access to modern laboratory equipped with everything needed for carrying out air– and moisture sensitive chemistry.

About the department

As KBFI is research only institution, the PhD candidate will be enrolled as a doctoral student to the nearby Tallinn University of Technology (Taltech). The candidate will have access to Taltech lectures, courses and academic resources at the full PhD curriculum capacity. Funding will be available for 4 years since the start of contract.

The PhD candidate will be integrated into the KBFI Organometallic chemistry research group and will be supervised by Dr Martin Jakoobi. The group maintains facilities for air-/moisture sensitive sample handling, sample preparation and fume hoods equipped with Schlenk lines and appropriate glassware to carry out manipulations with sensitive reagents. This PhD project will take advantage of the availability of various NMR spectrometers (200, 300, 360, 500, 600 and 800 MHz magnets) to assess the synthesis of various reagents, complexes and the outcomes of hydrogenation reactions. Additionally, the laboratory operates in-house developed *p*-H_2 hyperpolarization equipment that allows experimental workflows for which commercial instrumentation is not available.

(Additional information)

Interested candidates should contact Dr Martin Jakoobi at martin.jakoobi@kbfi.ee

References

1) Reimets, N.; Ausmees, K.; Vija, S.; Trummal, A.; Uudsemaa, M.; Reile, I. Parahydrogen hyperpolarized NMR detection of underivatized short oligopeptides. Analyst 2023, 148, 5407–5415, doi:10.1039/D3AN01345F.

2) Tokmic, K.; Markus, C. R.; Zhu, L.; Fout A. R. Well-Defined Cobalt(I) Dihydrogen Catalyst: Experimental Evidence for a Co(I)/Co(III) Redox Process in Olefin Hydrogenation. J. Am. Chem. Soc. 2016, 138, 11907−11913, DOI: 10.1021/jacs.6b07066

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3) Najera, D. C.; Fout, A. R. Iron-Catalyzed Parahydrogen Induced Polarization. J. Am. Chem. Soc. 2023, 145 (38), 21086–21095, DOI: 10.1021/jacs.3c07735.

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