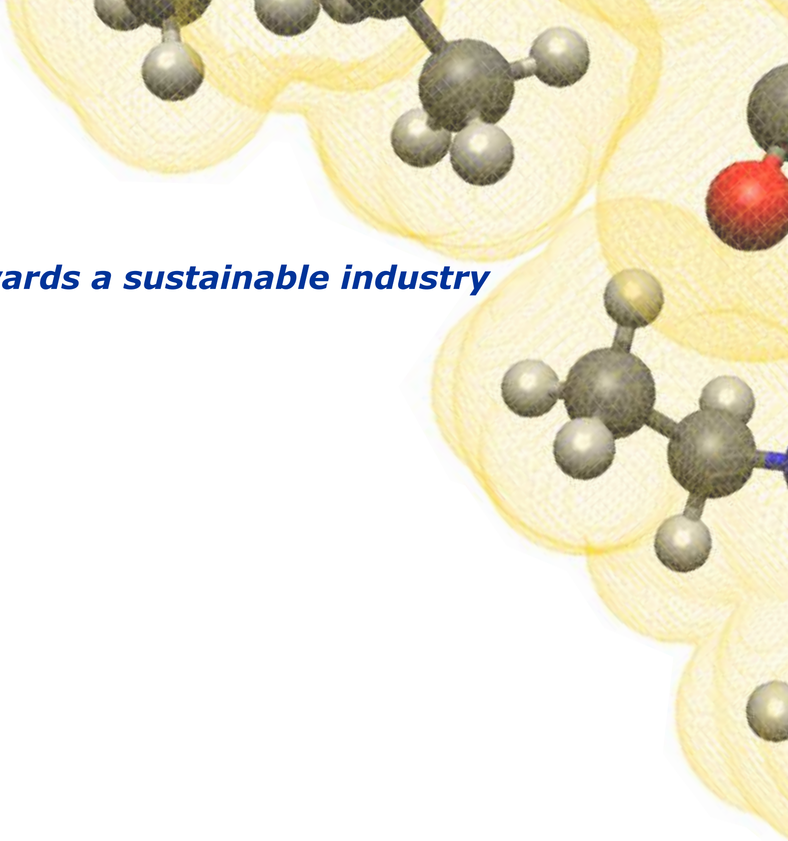
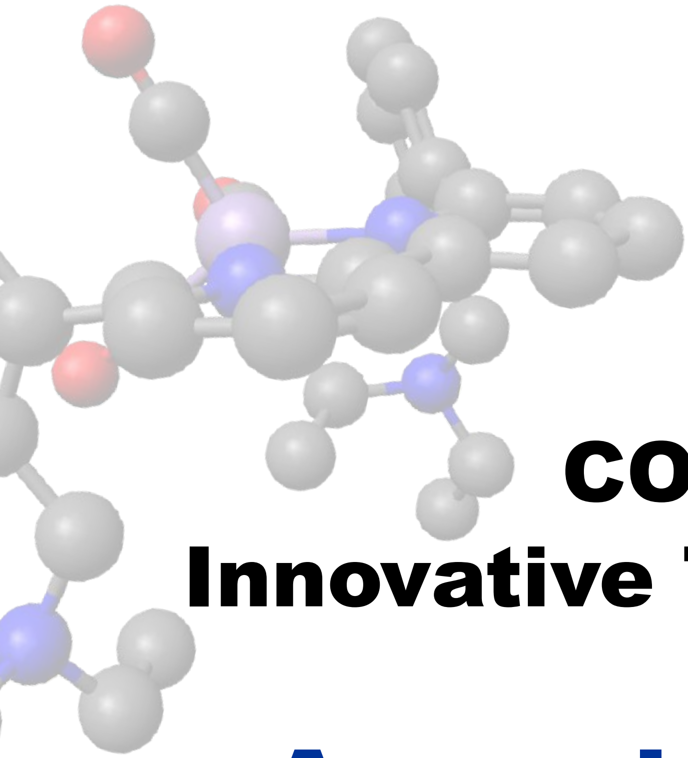
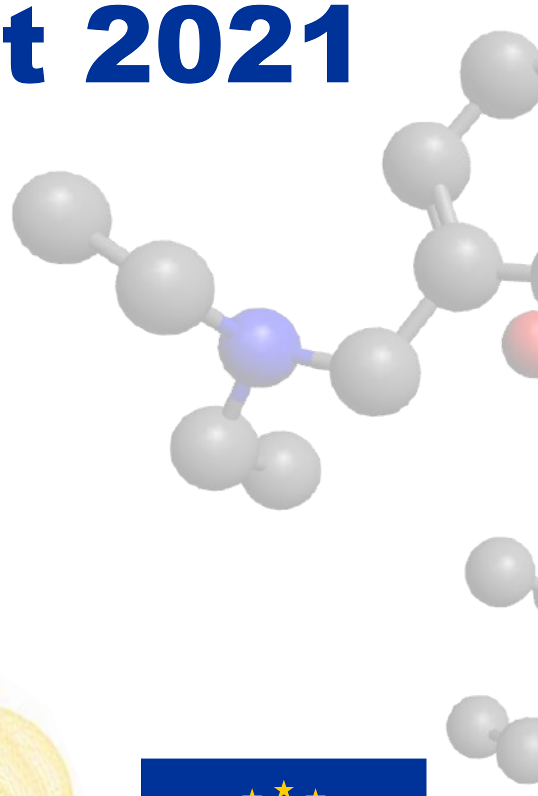


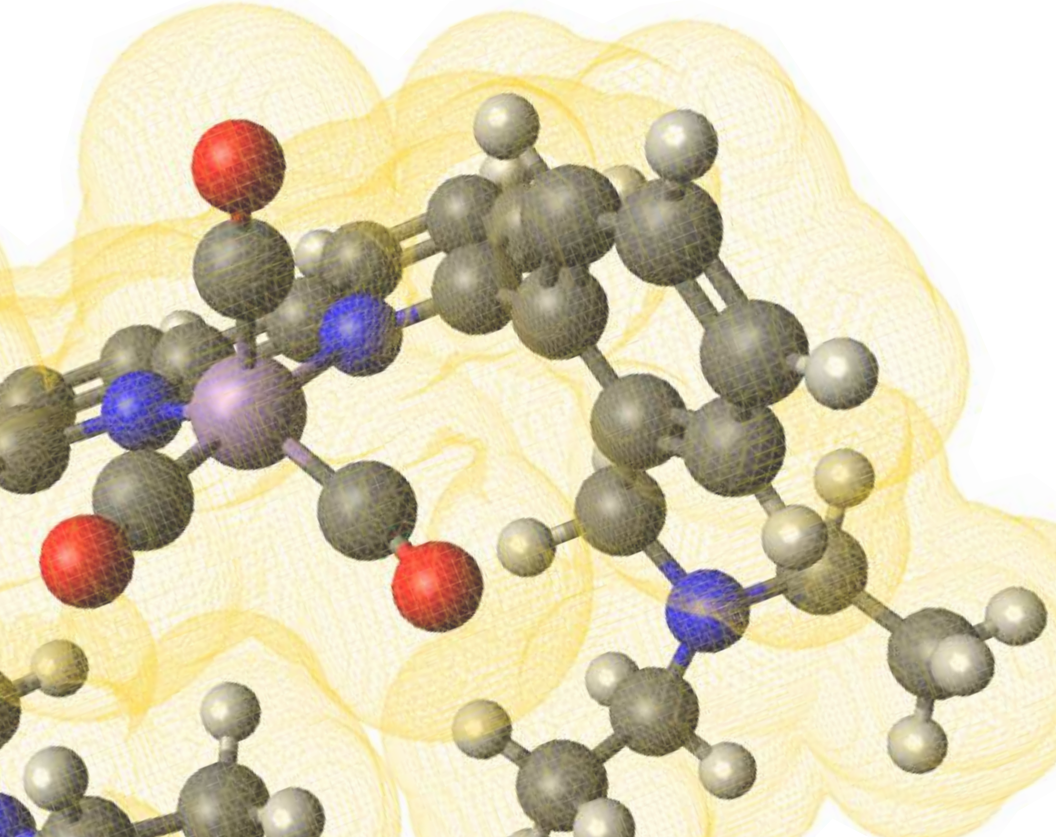
Cooperation towards a sustainable industry



CO_2PERATE Innovative Training Network

Annual Report 2021





Front Page:
The $Mn(dEAbpy)(CO)_3Br$ catalyst, a Mn bipyridine complex carrying *N,N′*-(([2,2′-bipyridine]-6,6′-diylbis(2,1-phenylene))bis(methylene))bis(*N*-ethylethanamine) (dEAbpy).
This type of catalyst is is used for the homogeneous electroreduction of CO_2 to CO and formic acid.
Illustration by M.-J. H. Halsør with compound files from M. Luthra.

CO_2PERATE Innovative Training Network
Horizon 2020 research and innovation programme - Marie Skłodowska-Curie grant agreement No. 859910
Contact address: Dept. of Chemistry, UiT The Arctic University of Norway, Tromsø, Breivika NO-9037 TROMSØ
co2perate.eu co2perate@uit.no @co2perate_ITN

CO_2PERATE ITN
Public Annual Report 2021

Table of contents

Overview

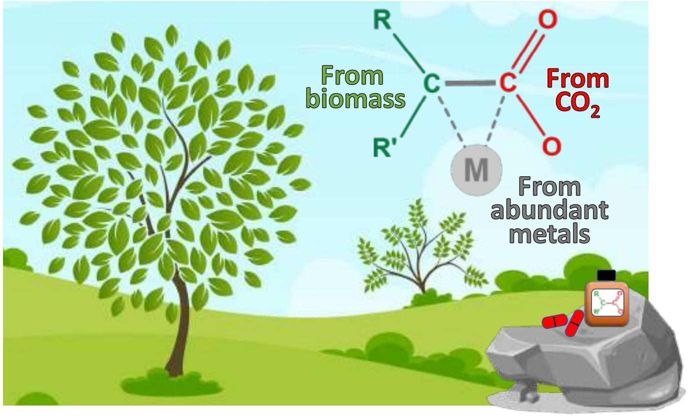
CO_2PERATE: Cooperation towards a Sustainable Chemical Industry

Hello again!

We are happy to present the second Annual Report of CO_2PERATE. By browsing this document, you will learn about CO_2PERATE's progress and activities in 2021, recent research highlights, and interviews with our Early-Stage Researchers (ESRs).

Who are we?

We are an Innovative Training Network (ITN), funded under the Horizon 2020 research and innovation programme - Marie Skłodowska-Curie grant agreement No. 859910. CO_2PERATE is composed of 10 Beneficiaries (3 industrial & 7 academic) and 2 Partners (see page 3 for all), across 6 European countries. Together we are training 15 skilled ESRs towards a PhD degree.



(Figure: K.H.Hopmann)

The CO_2PERATE organization is described on page 4 and a double-page feature showing a graphical overview of the whole network on page 18. ESRs that joined the network in 2021 will tell you more about themselves, their projects and the reasons why they joined CO_2PERATE from page 31.

What is our vision?

CO_2PERATE has a simple but essential vision: Training of a new generation of European researchers in the synthesis of indispensable molecules from sustainable carbon sources and with sustainable catalysts. This involves development of novel and industrially relevant methods for employing CO_2 as a carbon synthon, alongside other renewable biomass, catalysed by non-precious metals. Our research is described in more detail in our Research section (from page 5), including a list of our publications so far as well as highlights of the ongoing research (from page 8). As a part of their training, our ESRs are undergoing secondments which you can read about from page 25.

How can you find us?

Email us at co2perate@uit.no, or follow our daily life on social media (Twitter: @co2perate_ITN; Facebook: @co2perateITN or on our webpage co2perate.eu.

The 10 CO$_2$PERATE Beneficiaries

UiT The Arctic University of Norway

Stockholm University

Catalysis
Leibniz-Institut für Katalyse e.V.
LIKAT

University of Zurich UZH

EVONIK
POWER TO CREATE

UNIVERSITY OF OSLO

TOPSOE

AstraZeneca

ICIQ
Institute of Chemical Research of Catalonia

AARHUS UNIVERSITY

The 2 CO$_2$PERATE Partners

RUHR UNIVERSITÄT BOCHUM
RUB

UNIVERSITAT ROVIRA i VIRGILI

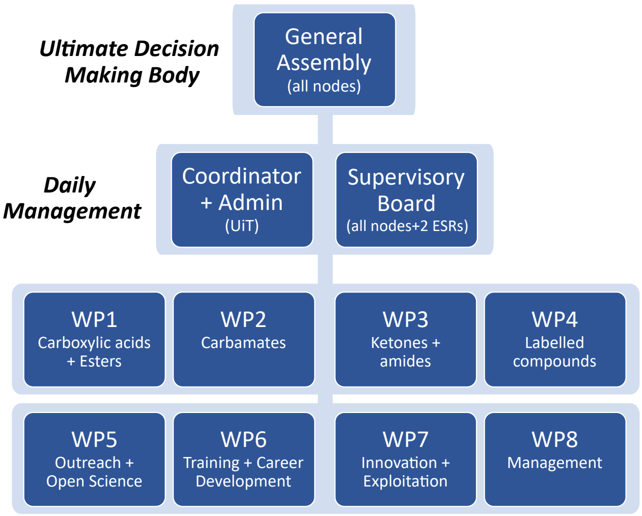
Overview

CO_2PERATE Organisation

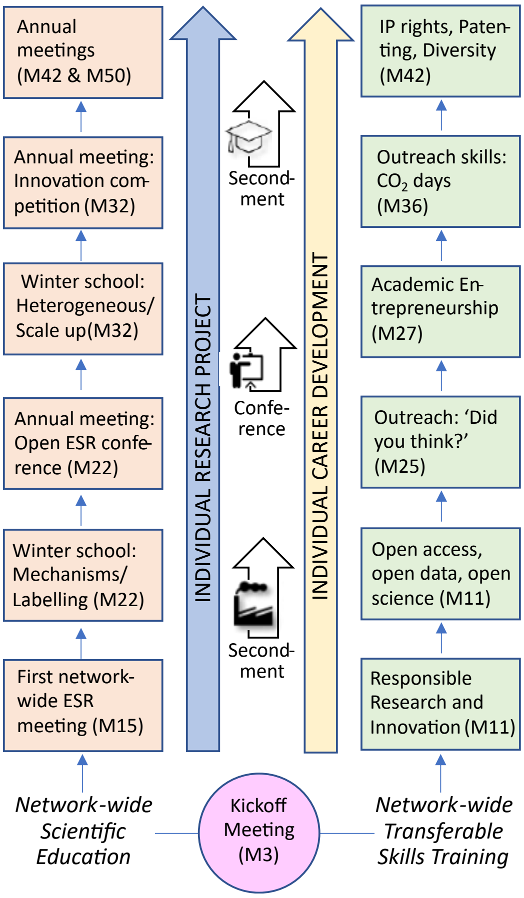
The CO_2PERATE project is funded by the European Commission from 2020 to 2024. CO_2PERATE comprises 10 beneficiaries and 2 partners in 6 European countries. 15 ESRs (PhD students) are part of the action.

The CO_2PERATE research focuses on developing reactions for sustainable conversion of CO_2 to products of higher value. CO_2PERATE has 4 research Work Packages (WPs), which represent the target molecules whose synthesis will involve CO_2 (see pages 5 and 6). 4 additional WPs oversee critical non-research task: WP5 is about Outreach, Dissemination & Open Science, while WP6 tackles Training & Career Development of our ESRs (see figure of training pillars). WP7 focuses on Innovation & Exploitation, and WP8 on Management.

CO_2PERATE Organization Structure



Organization of the CO_2PERATE project (figure K. H. Hopmann).



The CO_2PERATE training pillars (figure K. H. Hopmann)..

The CO_2PERATE ITN has established a General Assembly (GA), which includes all beneficiaries & partners and is the ultimate decision-making body. The daily implementation of the action is ensured by the Supervisory Board (SB), the ITN Coordinator (K. H. Hopmann) and the Project Manager (M.-J. H. Halsør).

CO_2PERATE project leader Kathrin H. Hopmann (left) and project manager Marie-J. H. Halsør (right, UiT).

Research

The research within the CO_2PERATE ITN is entirely focused on the sustainable conversion of CO_2, with the goal of generating products of higher value. Depending on the type of compounds that we wish to study the synthesis of, four work packages have been designed.

WP1: Carboxylic acids and Esters

WP1 aims to develop "*efficient non-precious metal catalysts for the formation of carboxyl and ester motifs from CO_2 and sustainable starting materials*"[1]. Seven ESRs participate in this project with ESRs 1-4 developing both homogeneous and heterogeneous catalysts. ESRs 5, 13 & 14 are tasked with the computational analyses as well as theoretical studies related to the reactions studied experimentally.

WP2: Carbamates

In this work package, ESRs 6 & 7 focus on the efficient formation of oxazolidinones using homogeneous catalysis, with ESR3 investigating immobilized catalysts. They are also exploring enantioselective reactions, with the help of ESR8 for computational mechanistic studies.

WP3: Amides & Ketones

Carbonylation and aminocarbonylation processes leading to amides and ketones from CO_2 are studied by ESRs 3, 9 & 15, who are developing non-precious catalysts, as well as ESR10 and 14 for the computational studies. This work package includes work on the reduction of CO_2 to CO (ESRs 15 & 14), as a part of aminocarbonylation processes.

WP4: Labelled compounds

The aim of this package is to develop "*New versatile technologies for the isotopic labelling of chemicals, pharmaceuticals, and proteins with* $^{11}CO_2$, $^{13}CO_2$, *and* $^{14}CO_2$"[1]. ESRs 9, 12 & 11 are doing the experimental work with ESRs 5 & 8 tasked with computational studies.

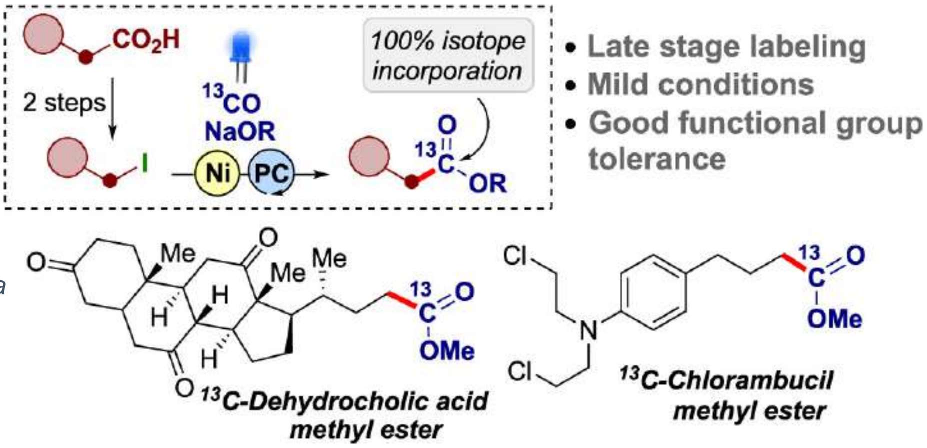
References

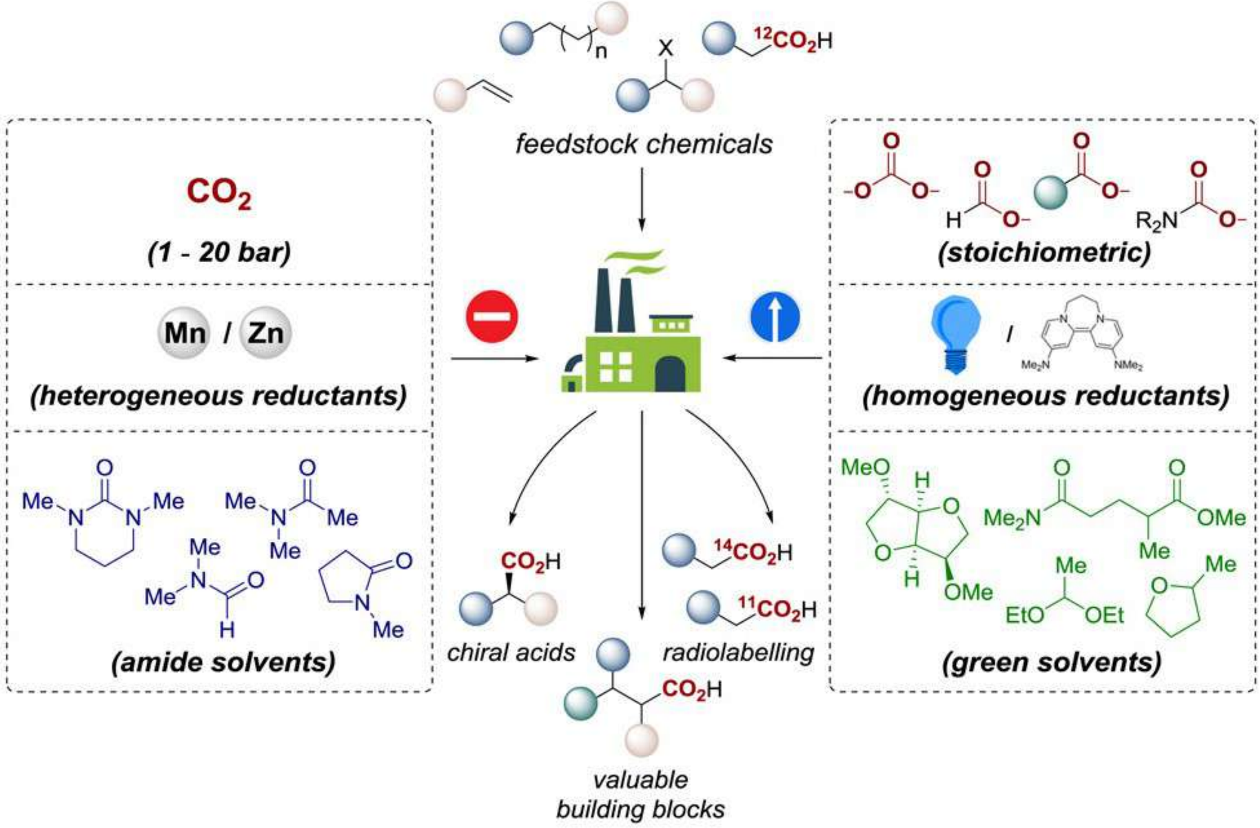
1. CO_2PERATE Grant Agreement,
Annex 1B– Description of the Action

Research

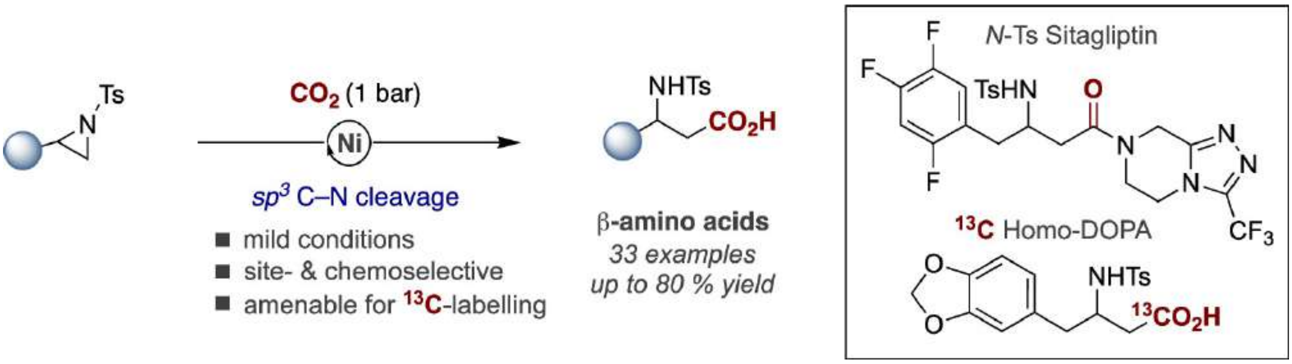
Publications

ESR9 Stephanie Ton and collaborators present “a direct synthetic route allowing for full carbon isotope replacement via a nickel-mediated alkoxycarbonylation”[1].





The group from ICIQ, involving ESR1 Dmitry Zimin and ESR11 Julien Lyonnet, presents in a review “a critical view of the catalytic carboxylation arena, discuss the current limitations, and explore how the most recent advances offer tantalizing hints of how these challenges may be addressed”[2].



ESR1 Dmitry Zimin participated in the paper showing “A Ni-catalyzed reductive carboxylation of N-substituted aziridines with CO$_2$ at atmospheric pressure”[3].

1. **Ton, S. J.**; Neumann, K. T.; Nørby, P.; **Skrydstrup, T.** Nickel-Mediated Alkoxycarbonylation for Complete Carbon Isotope Replacement. *J. Am. Chem. Soc.* **2021**, 143, 17816-17824. DOI: 10.1021/jacs.1c09170.
2. Davies, J; **Lyonnet, JR**; **Zimin, DP**; **Martin, R.** The road to industrialization of fine chemical carboxylation reactions. *Chem* **2021**, 7, 2927-2942. DOI: 10.1016/j.chempr.2021.10.016.
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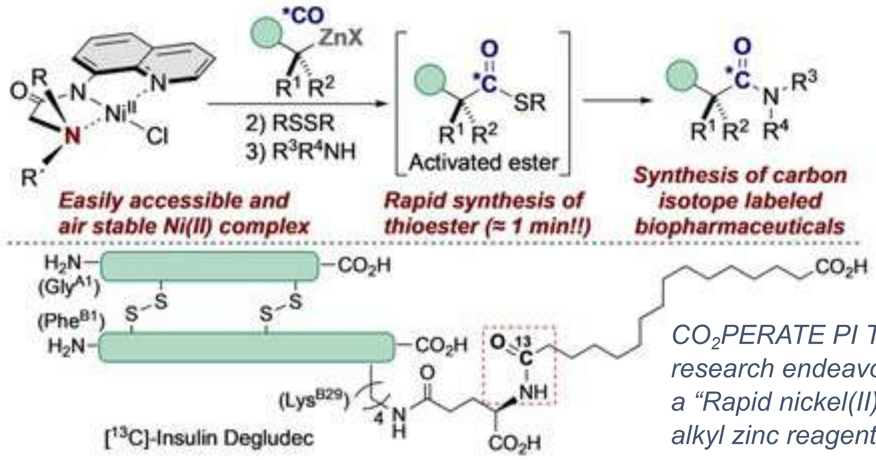


CO$_2$PERATE PI Troels Skrydstrup led the research endeavour leading to the presentation of a “Rapid nickel(II)-mediated thiocarbonylation of alkyl zinc reagents”[4].

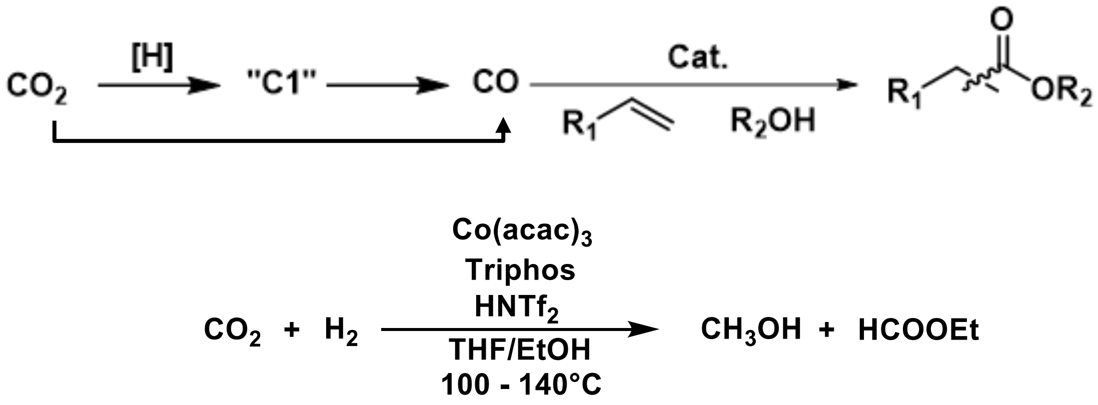
A closer look at...

WP1, PROJECT 13
LIKAT
WEIHENG HUANG

Project 13, titled “Catalytic alkoxycarbonylation reactions of unsaturated hydrocarbons with CO_2 “(WP1, “Carboxylic acids and esters from CO_2”), is supervised by Prof. Matthias Beller in Leibniz Institute for Catalysis (LIKAT). The main objective of the project is replacing toxic CO with CO_2 for industrially relevant alkoxycarbonylation reactions with olefins to give esters and related compounds. The targeted products are important intermediates for the production of many daily life products ranging from flavour and fragrances, pharmaceuticals to high performance polymers. To make the current processes for esters more sustainable, non-noble metals such as Fe and Co are primarily adopted for new homogeneous catalyst development.

In project 13, a two-step strategy is proposed for accomplishing these challenging goals: first CO_2 reduction and as a second step alkoxycarbonylation of olefins with in-situ generated CO from the first step. Alcohols are the ideal reducing agent for this reaction, but so far only few literatures report such transformations.[1] Alternatively, hydrogen gas can be chosen as reductant for carbon dioxide, because CO could be obtained directly via reverse water gas shift reaction.

What’s more in this project? Other interesting products from CO_2 like formic acid, methyl formate and formaldehyde are also evaluated as the starting material for carbonylation reaction with olefins.[2]



$$CO_2 + H_2 \xrightarrow[\substack{\text{THF/EtOH} \\ \text{100 - 140}^\circ\text{C}}]{\substack{\text{Co(acac)}_3 \\ \text{Triphos} \\ \text{HNTf}_2}} CH_3OH + HCOOEt$$

The overall process of the two-step strategy for the alkoxycarbonylation reaction and the catalyst system composed of CO_2 with cobalt-triphos (figure: W. Huang).

However, also these reactions are still quite challenging. In all the mentioned reactions, our priority is reducing CO_2 with high selectivity that means preventing unsaturated hydrocarbons to be reduced by H_2. In all these CO_2 reductions, water is a by-product after the carbonylation reaction. That suggests the catalyst should be moisture tolerant. To guarantee the reactivity of carbonylation reaction, our reactions are essentially carried out under non-basic conditions which would not inhibit the formation of metal hydride, especially for non-noble metals. Considering these restrains, different catalysts were synthesized, combined and tested. One of the representative examples is the cobalt-triphos catalyst system.[3,4]

Here, CO_2 is reduced to methanol and ethyl formate with ethanol in the presence of cobalt-triphos catalyst with strong acid $HNTf_2$. According to detailed DFT calculations, at the beginning CO_2 inserts in to $[P^3Co\text{-}H]+$ hydride complex and then reacts with H_2 to form formic acid.[3,4] Based on the experimental and DFT results, we introduced some efficient alkoxycarbonylation palladium catalysts into the reaction. At present the search for more active and selective catalysts is continued in this project.

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2. L. Wu, Q. Liu, R. Jackstell, M. Beller, 2014. 53, 6310-6320. DOI: 10.1002/anie.201400793

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Early-stage researcher Weiheng Huang with his main supervisor Matthias Beller (LIKAT) and his co-supervisors Cristina Nevado (UZH) and Robert Franke (EV).

A closer look at...

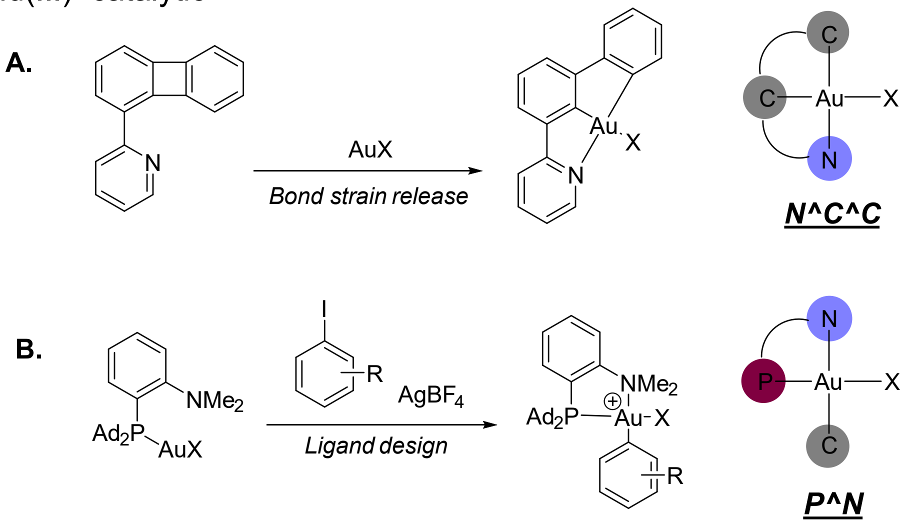
WP2, PROJECT 7
UNIVERSITY OF ZÜRICH
DORIANE CHAUVIN

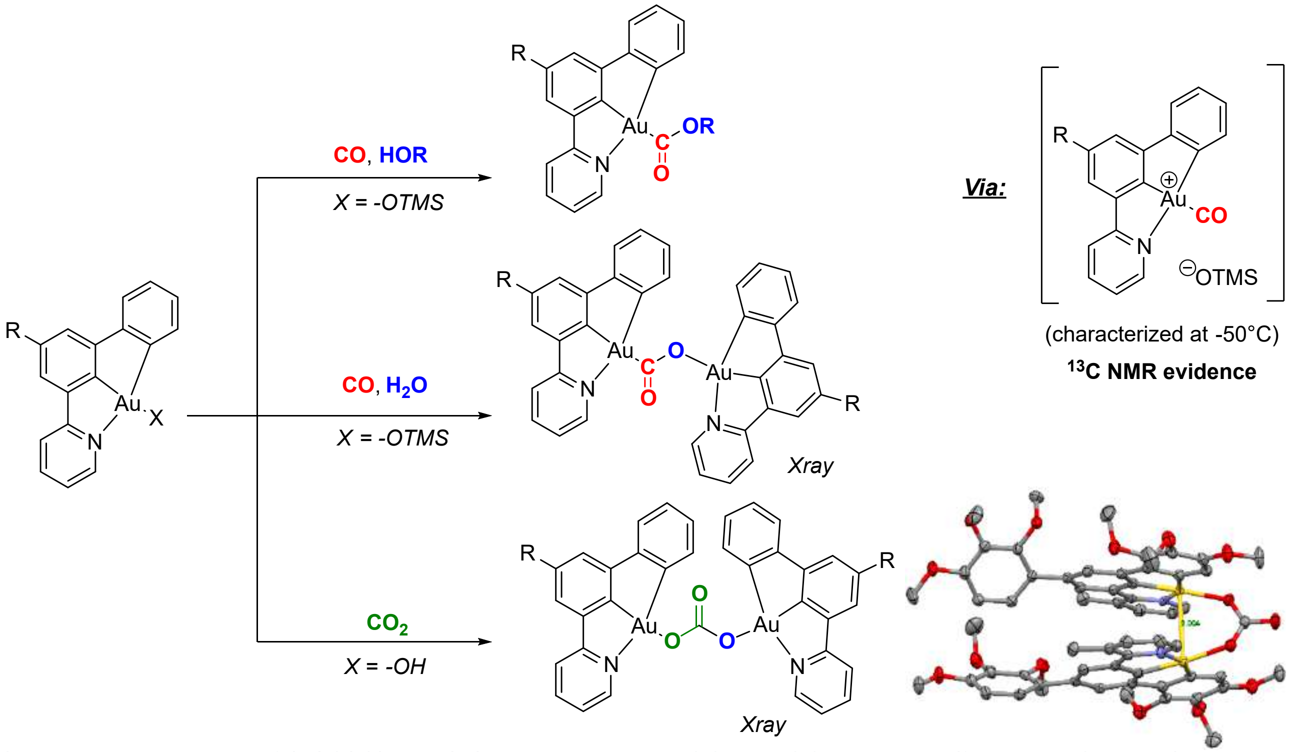
Project 7, titled “Multicomponent functionalization of π-systems incorporating CO_2”, is conducted at the University of Zürich under the supervision of Prof. Cristina Nevado. The research focus relies on the development of new homogeneous catalysed transformations targeting the incorporation of carbon monoxide and carbon dioxide into organic molecules.

As starting point for these endeavours, our group aims to gain fundamental understanding of the reactivity of COx within specifically designed ligand templates stabilizing the metal complexes of choice for these transformations. In this context, there is a particular interest in gold, given its unique properties in the activation of C-C unsaturated bonds together with its tolerance to a wide range of functional groups[1,2]. Further, and due to its reluctance to undergo oxidative addition[3], gold catalysis has long been restricted to gold(I) or gold(III) catalytic cycles involving no change in the oxidation state of the metal.

This paradigm has been recently revisited and the chemistry community has witnessed a growing renewed interest into this field. Ligand design, photochemistry or strain release have turned out to be elegant and efficient solutions to address the challenges associated to the development of transformations involving gold(I)/gold(III) turnovers[3]. Several mono- and bis-cyclometallated gold(III) complexes have been developed and studied within our group (Scheme 1).

Scheme 1. Relevant examples of various gold complexes accessible via oxidative additions (N^C^C4,5, P^N6). Figure by D. Chauvin.



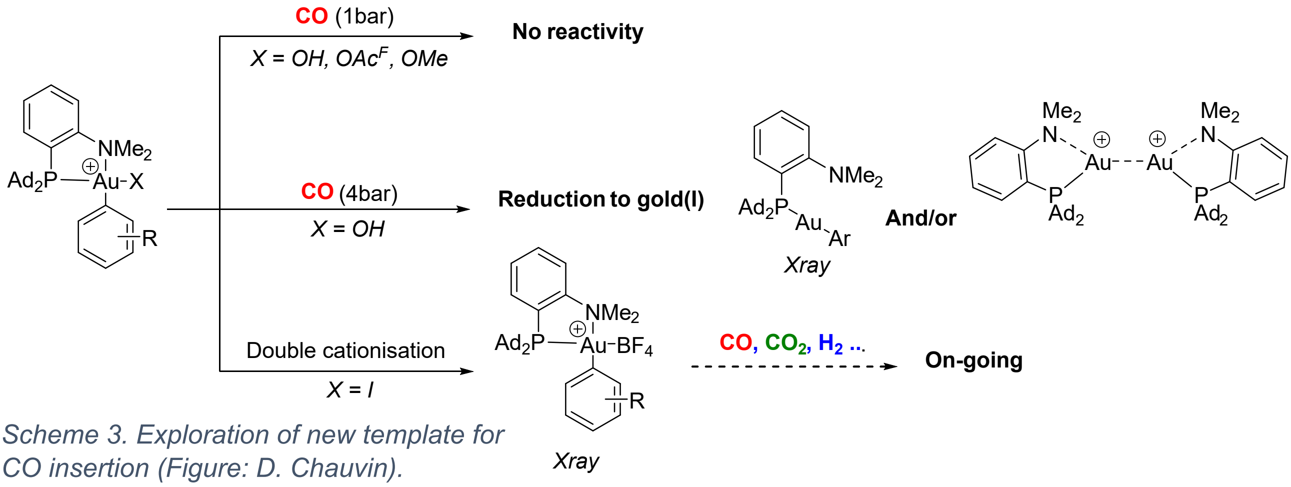


Scheme 2. Reactivity of (N^C^C) gold(III) complex toward CO and CO_2 insertion (figure: D. Chauvin).

Despite its attractive properties, the reactivity of gold toward CO and CO_2 activation remains underexplored. Our group recently reported the CO insertion under mild conditions to access a novel class of gold(III) carboxylates[7] (Scheme 2). The (N^C^C) pincer ligand proved to efficiently stabilize reactive complexes, postulated to be key intermediates in catalytic processes. This enables us to gain fundamental mechanistic insight for further developments.

More investigations for COx insertion and the exploration/design of new templates are currently on-going (Scheme 3). The P^N template exhibits attractive features for the development of catalytic cycles. Several attempts of CO and CO_2 insertion under mild conditions (one atmosphere) did not show any reactivity, while increasing the pressure led to the reduction/decomposition of the complex. Nevertheless, synthesis and crystallization of specific sensitive species lay out the ground for additional research on activation of hydrogen, carbon monoxide and so on.

Research



Scheme 3. Exploration of new template for CO insertion (Figure: D. Chauvin).

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DOI: 10.1039/D1SC03814A

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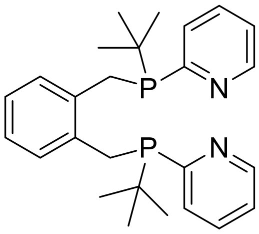
Early-stage researcher Doriane Chauvin with her main supervisor Cristina Nevado (UZH) and her co-supervisors Belén Martín-Matute (SU) and Esben Taarning (HT).

WP3, PROJECT 14
EVONIK
JIALI LIU

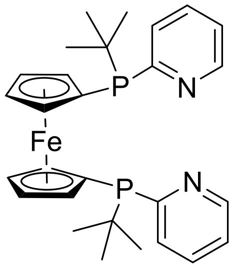
A closer look at…

Project 14 “Theoretical studies on catalytic alkoxycarbonylation and carbonylation reactions with CO_2” is a part of WP1 (“Carboxylic Acids and esters from CO_2”) and WP3 ("Amines and ketones from CO_2"). It aims to investigate the reaction mechanism of alkoxycarbonylation and carbonylation using CO_2, and to further optimize and design better catalytic systems. But we firstly explore the mechanism of alkoxycarbonylation using CO, which will provide insight for our studies of CO_2. These orienting calculations represent the starting point for our further mechanistic investigations.

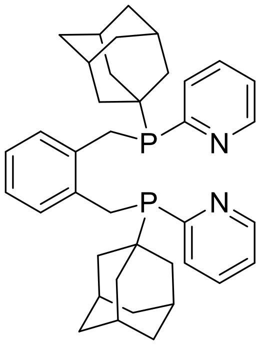
Alkoxycarbonylation of inert alkene was a challenging topic, until Beller’s group synthesized and introduced the 1,2-bis((tert-butyl(pyridin-2-yl)-phosphanyl)methyl)benzene (**L1**, Pytbpx) ligand with Pd precursor into methoxycarbonylation of tetramethylethylene[1]. Though the later described ferrocene[2] (**L2**) and adamantyl[3] **(L3)** ligands also show excellent activity, we focus on the pytbpx ligand because investigations into its stability and optimizations of ligand synthesis make this the most promising candidate at present. In particular, we ask ourselves the following questions in this project: How do the isomerization and methoxycarbonylation take place using the pytbpx ligand? And how to further optimize the catalytic system?



L1

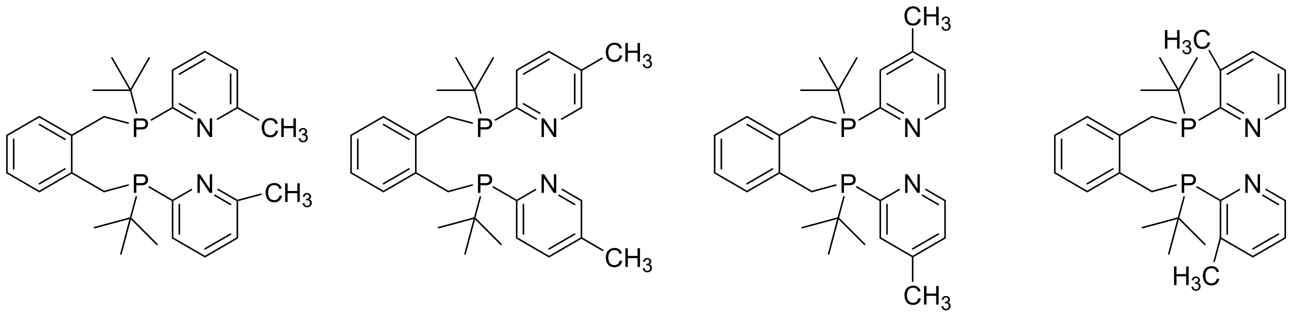


L2



L3

Several excellent ligands for methoxycarbonylation of alkenes (figure: Jiali Liu).



L1-3-CH$_3$ **L1-4-CH$_3$** **L1-5-CH$_3$** **L1-6-CH$_3$**

Selected substituent ligands (figure: J. Liu)

For solving above questions. We explored this reaction pathway firstly, whereby from a collaboration with my colleague Stefan Müller, who is carrying out an experimental doctoral thesis on this topic at Evonik, data from catalysis experiments are available with which I can directly compare my results from the quantum chemical calculations. Furthermore, the substituent effect is also considered, and it can affect the stability of vital transition states and intermediates to further influence the catalyst reactivity and reaction selectivity. So, we explored the Gibbs free energy profile with the CH$_3$ group at 3-,4-, 5- and 6- position of the pyridine moiety of the ligand. Calculated Gibbs free energy barriers are almost consistent with experimental results and one of the substituted complexes show better catalytic performance than the original one (**L1**) both in the theoretical as well as in the experimental study. However, there is also a significant discrepancy between the experimental data and the theoretical predictions for the **L1-4-CH$_3$** ligand. We are currently investigating the reasons for this deviation.

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Early-stage researcher Jiali Liu with her main supervisor Robert Franke (EV) and her co-supervisors Annette Bayer (UiT) and Troels Skrydstrup (AU).

A closer look at...

WP4, PROJECT
ASTRAZENECA
KIM S. MÜHLFENZL

Project 12 is titled" Development of Late-Stage and Rapid Carboxylation Techniques with $^{14}CO_2$ Drug Development Programs" and is part of WP4 ("Labelled Compounds from CO_2"). The goal of this project is the expansion of the methods available for the late-stage ^{14}C-labeling of bioactive and pharmaceutically relevant molecules.

Carbon-14 (^{14}C) is a long-lived radioisotope (half-life = 5730 years) of carbon. In general, the incorporation of a radioisotope into a compound increases the sensitivity and ease of detection of the compound in both in vitro and in vivo. As a result, carbon-14 labelling is an important tool for investigating metabolite profiles and determining the pharmacological and toxicological effects of a drug candidate.[1] For this purpose, the label is incorporated into a metabolically stable position, preferably located in the core of the molecule, to prevent metabolic cleavage of the label. However, there are only a few commercially available starting materials, including $^{14}CO_2$ that can be used as a source for radiolabelling. This often leads to a modified synthetic pathway compared to the one previously developed for the unlabelled compound. To reduce radioactive steps and to save time and money, late- or even last-stage labelling techniques are preferable.

Carboxamides are prevalent in bioactive molecules and pharmaceuticals and often represent a metabolically stable position. Consequently, aminocarbonylations constitute significant reactions for the synthesis of pharmaceutically relevant molecules. Utilizing stochiometric amounts of labelled CO, these techniques can be also used for carbon isotope labelling.

In 2019, a method for the aminocarbonylation of inactivated alkyl iodides at ambient temperature enabled by visible-light and palladium catalysis in the presence of stoichiometric amounts of (labelled) CO was developed. It was found that this method also worked well for the carbonylation of aryl iodides at ambient temperature.[2]

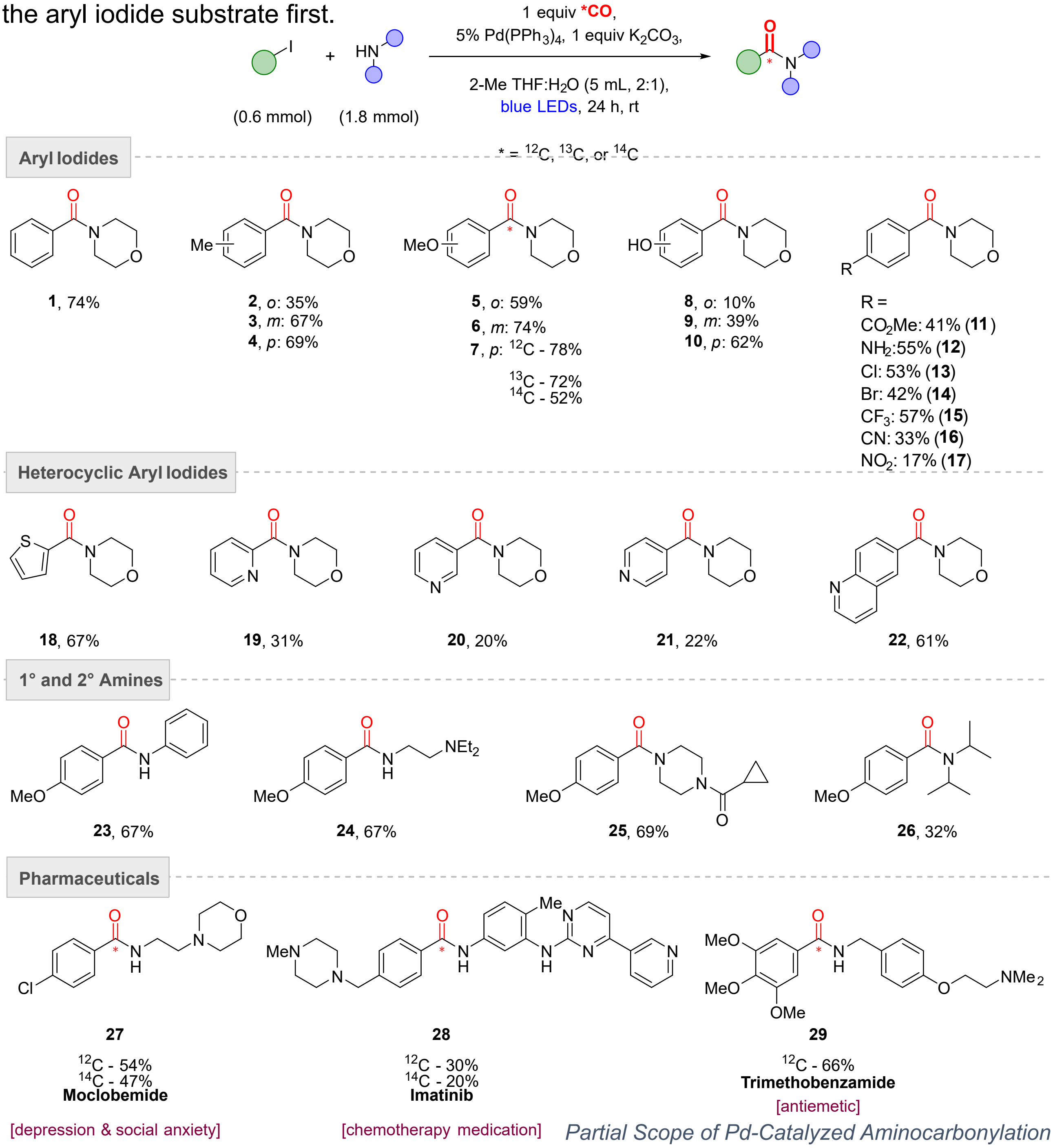
Inspired by this work, we investigated the visible-light enabled and palladium-catalysed aminocarbonylation of aryl iodides at ambient temperature in the presence of stoichiometric amounts of CO. Initial control and screening experiments, including catalyst, solvent, scale, and concentration, were carried using 4-iodoanisole and morpholine as model substrates. The reaction was conducted in a two-chamber glassware. This allows ex-situ generation of stoichiometric amounts of (labelled) carbon monoxide from the solid precursor, COgen, which can then diffuse into the reaction chamber.[3,4]

Research

Utilization of (labelled) COgen allows for an easy transfer from unlabelled to labelled reaction.

With the optimized conditions in hand, the scope of this aminocarbonylation was explored (see the presented reaction scheme), investigating the generality of the aryl iodide substrate first.

The conditions tolerate a wide range of functional groups and both electron-deficient and -rich aryl iodides undergo reaction (**1-17**). In general, lower yields were observed when switching from para- to meta- and eventually ortho-substitution most likely due to steric hindrance.



Partial Scope of Pd-Catalyzed Aminocarbonylation of Aryl Iodides. (Figure: K. Mühlfenzl)

A notable feature of this method is that heterocyclic aryl iodides can serve as substrates (**18-22**).

Next, the scope of the aminocarbonylation with respect to the nature of the amine was investigated. 1-iodo-4-methoxybenzene performed well with a range of primary and secondary amines (**23-26**). However, the reaction has shown to be sensitive to steric hindrance, as in the case of diisopropyl substitution, providing the corresponding product **26** in a relatively low yield. In addition, amines with low nucleophilicity have shown to be challenging to the method.

To further demonstrate synthetic utility, pharmaceutical relevant compounds (**27-29**) were isolated in good yields. Lastly, the reaction conditions were applied to C-14 labelling. To keep the radioactive waste relatively low, a dilution of 5% ^{14}COgen in unlabelled COgen was used and [^{14}C]-**7**, [^{14}C]-**27**, as well as [^{14}C]-**28** were successfully synthesized.

Using visible-light and palladium catalysis, a versatile method for the late-stage aminocarbonylation of aryl iodides was established. Noteworthy, this method works with carbon monoxide as limiting reagent and at ambient temperature. This provides an alternative for late-stage labeling amides, especially of temperature-sensitive compounds. The conditions tolerate a wide range of functional groups, including electron-deficient and -rich aryl iodides as well as amines with varying nucleophilicity, and provide the substrates with moderate to good yields. In addition, ^{14}C-labeled substrates were successfully synthesized.

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Early-stage researcher Kim Saskia Mühlfenzl with her main supervisor Chad Elmore (AZ) and her co-supervisors Annette Bayer (UiT) and Troels Skrydstrup (AU).

The CO2PERATE Innovative Training Network


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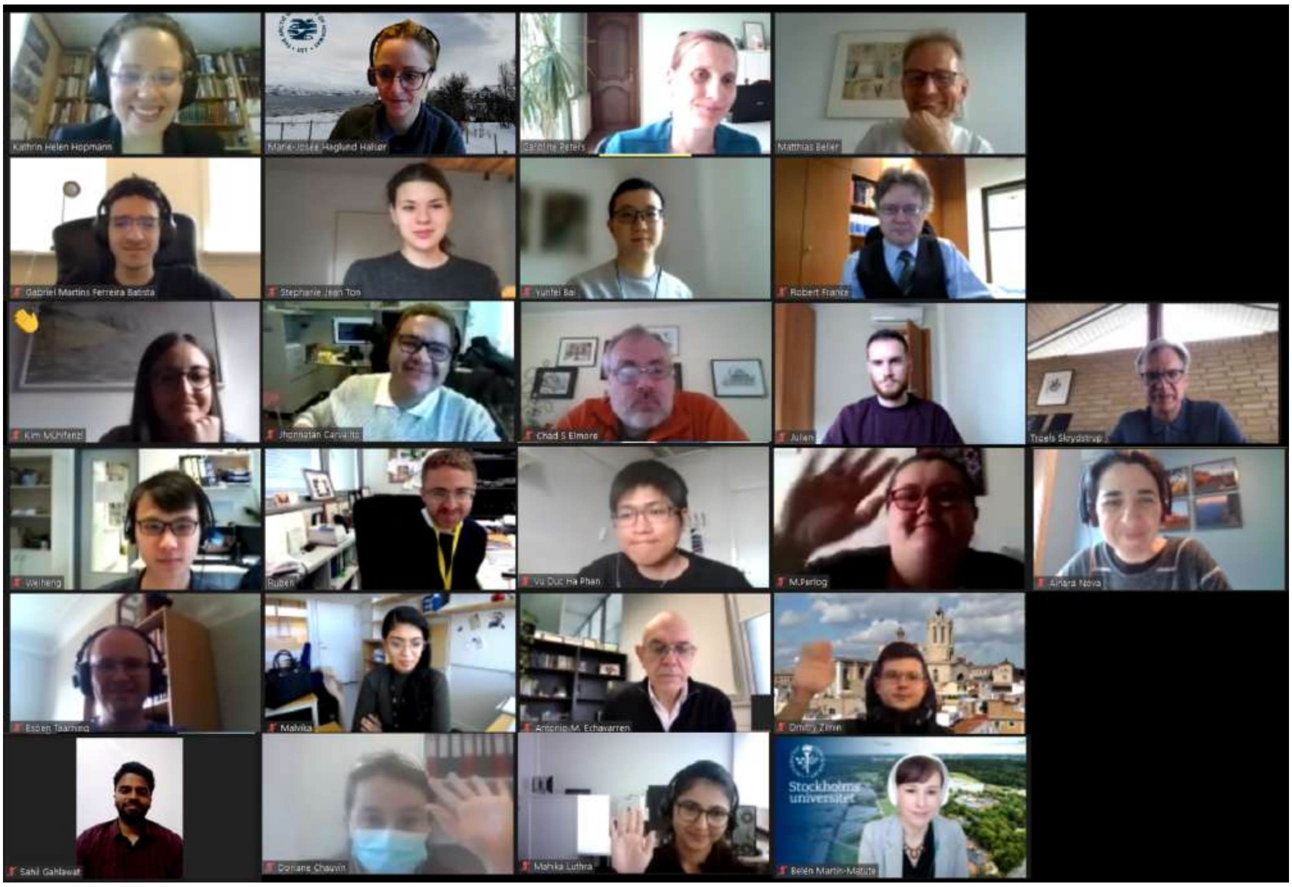
Activities

2021 at a glance:

We started 2021 with 12 out of 15 ESRs and the hope that the pandemic would be over soon. Our main goal for 2021 was to recruit the rest of the ESRs, have at least one physical gathering, and complete the Mid-Term Check Meeting (MTC) with the Research Executive Agency from the European Commission. We managed to do all three, with the last ESRs recruited during the summer. Unfortunately, ESR15 (LIKAT) had to leave the ITN around the same time; a new candidate for the position has been found. We had the MTC Meeting in April, and the ESRs met physically for the first time at the occasion of the Winter School 2021, which was organised in collaboration with the NordCO$_2$ consortium in November, at the University of Oslo.

In addition to this, the ESRs met digitally every first Wednesday of the month at the ESR ITN meetings. The Supervisory Board (SB) also met in 2021.

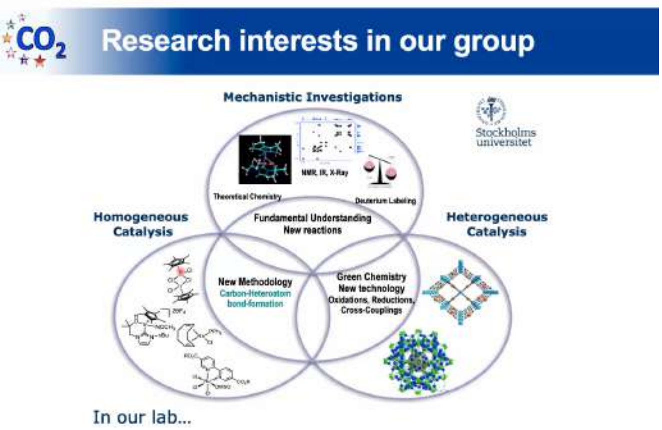


The ITN at the MTC meeting, together with PO Caroline Peters.

Research Executive Agency Mid-Term Check Meeting

29TH - 30TH APRIL
DIGITAL MEETING

All CO$_2$PERATE members gathered to meet our Project Officer (PO) Caroline Peters from the European Commission (Research Executive Agency, REA) to present our ITN and discuss our progress. Taking advantage of this occasion, the ITN met the day before, without our PO to catch up. While the meeting was originally scheduled to be a physical meeting in Tromsø, it was apparent early on that the travelling restrictions would not allow for it, and we planned for a digital meeting instead.



CO$_2$ Research interests in our group

In our lab...

Pr. Martín-Matute presenting her research group at Stockholm University on the first day of the meeting.

AstraZeneca

Not a straight line – my career journey

Per-Ola Norrby
Data Science & Modelling, Pharm. Sci., R&D, AstraZeneca Gothenburg

29 April 2021

Pr. Norrby's title slide for his "Speaking from experience..." presentation.

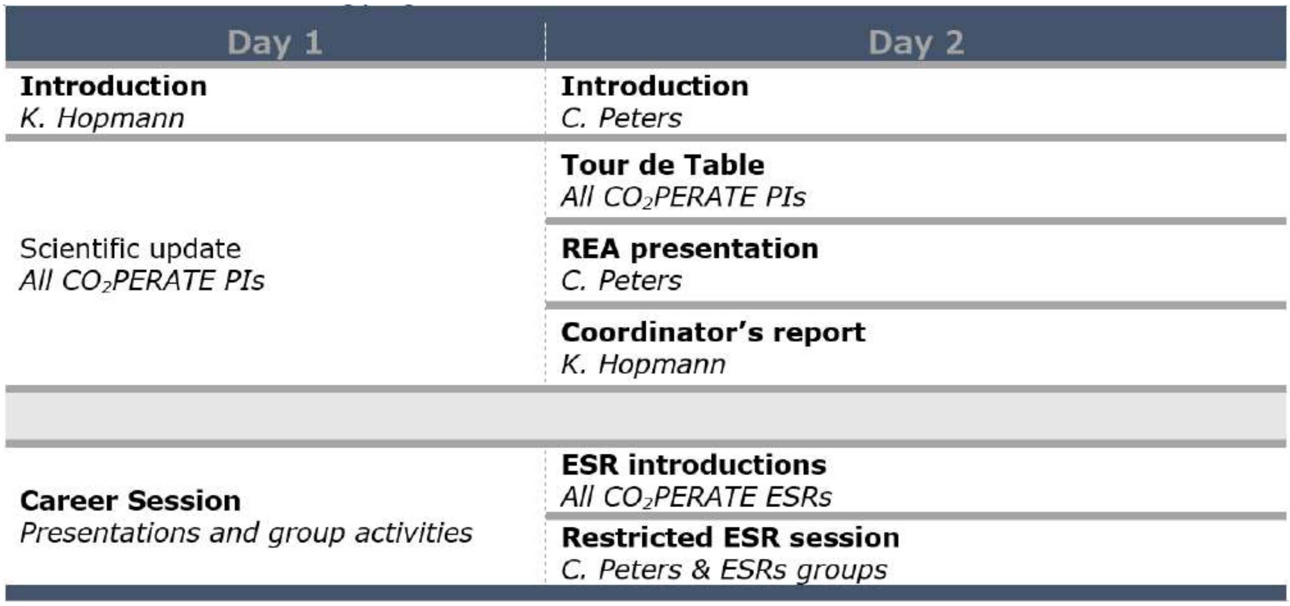
We began the first day with a few words from our leader, Prof. Kathrin Hopmann (the Coordinator), followed by a scientific update from all the Principal Investigators (PIs) of the ITN. After a lunch break, we focused our attention on the career development of our ESRs, with group activities and presentations. The ESRs had to think about topics such as “What is your career goal” and “How do you get there”. Presentations were centred around the theme of “Speaking from experience…”, and we got to hear about the career paths of Prof. Per-Ola Norrby (AZ), Dr. Malvika Sardana (AZ) and Prof. Matthias Beller (LIKAT). The presentations were scheduled between the two group activities, so that the ESRs had the opportunity to shape more informed answers. After the session, all the ITN gathered once more for a general discussion.

Activities

On the second day, we had an introduction from our PO, followed by presentations from all the beneficiaries and partner organisations of the ITN. Everyone briefly presented their research groups and their role in the consortium. After that, it was the PO's turn again, who talked to us about monitoring the project implementation and why there is a mid-term check. This talk was followed by the coordinator's report, given by Prof. Hopmann. She presented the ITN as a whole and the progress that was made in various areas such as recruitment, management, and the status of deliverables & milestones.

After lunch, it was time for the ESRs to present themselves, before heading into group meetings with the PO. This was the occasion for them to discuss with the REA representative about their experience within the ITN. The restricted session with the ESRs was followed by one with the Coordinator. Once the restricted sessions were over, the ITN gathered one last time for feedback from the REA and open discussion.

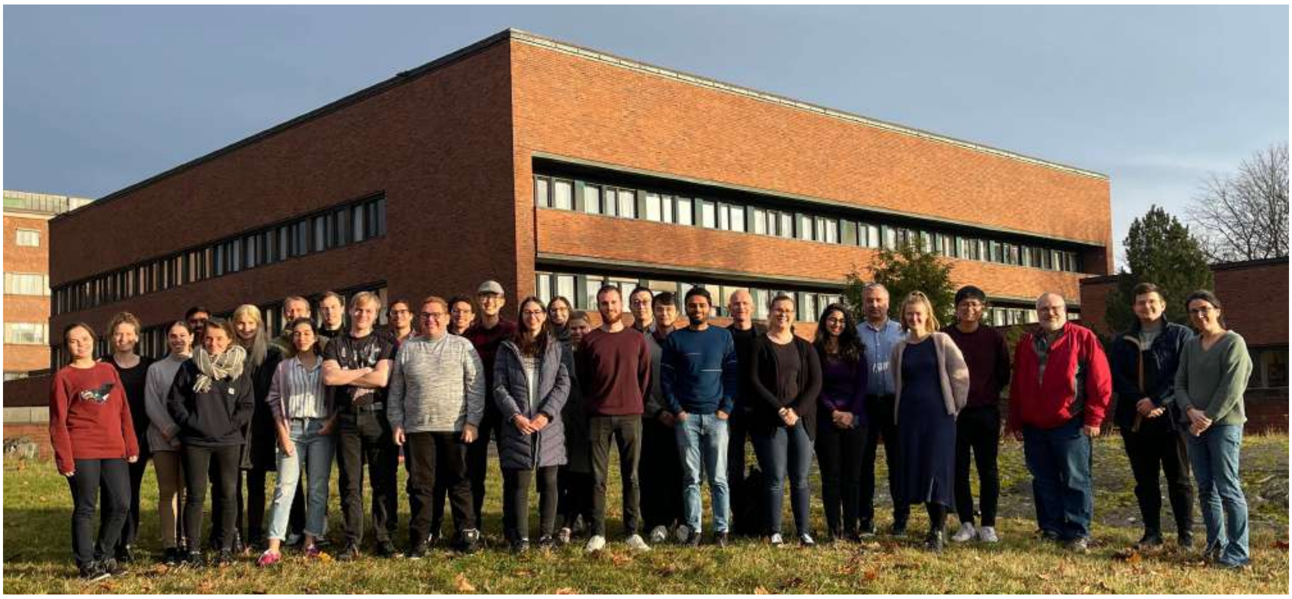
Overview of the MTC Meeting programme



Day 1	Day 2
Introduction *K. Hopmann*	**Introduction** *C. Peters*
Scientific update *All CO$_2$PERATE PIs*	**Tour de Table** *All CO$_2$PERATE PIs*
	REA presentation *C. Peters*
	Coordinator's report *K. Hopmann*
Career Session *Presentations and group activities*	**ESR introductions** *All CO$_2$PERATE ESRs*
	Restricted ESR session *C. Peters & ESRs groups*

Winter School 2021

22ND – 24TH NOVEMBER
UNIVERSITY OF OSLO, NORWAY



The CO_2PERATE ESRs together with NordCO_2 students at the Winter School 2021, in front of the Natural Sciences building of the University of Oslo (photo: M.-J. H. Halsør).

CO_2PERATE collaborated with the NordCO_2 consortium to organise the 2021 Winter School, which took place over the course of three days from the 22nd to the 24th of November 2021. The focus of the school was on the "Mechanisms of CO_2 activation" as well as "Isotopic labelling".

The course consisted of digital lectures in the mornings and practical sessions in the afternoon.

The winter School was the very first physical meeting across the ITN after almost two years of working together, and a much-awaited occasion for socializing.

Participants were distributed in groups for the afternoon pratical sessions. Special attention was given to blend the students according to their institutions and competences.

ITN ESR Meetings

FIRST WEDNESDAY OF THE MONTH DIGITAL MEETINGS

Networking without mobility is our challenge, and we are keeping contact with our Early-Stage Researchers as best as we can. They meet digitally each month to catch up and discuss various topics they have prepared beforehand, such as a session on CO2 reduction in the presence of olefins (without a base!) or planning an escape room event for future gatherings.

Supervisory Board Meetings

15TH FEBRUARY
7TH JUNE
10TH NOVEMBER
DIGITAL MEETINGS

The CO$_2$PERATE Supervisory Board (SB) met 3 times in 2021 to discuss the progress within the Work Packages, recruitment, and the ITN extension – which was approved by the REA, thus giving us until July 2024.

Amongst the decisions taken by the SB was the creation of the IP register of ideas for the ITN, led by AZ.

The SB also worked on the updated secondment schedule for the ESRs, considering the travel restrictions, new hires, and the ITN extension.

Finally, it was decided that C. Elmore (AZ) will replace T. Skrydstrup (AU) as SB leader for 2022. New ESR representatives were also elected, with G. Kriticou (UZH) and M. Luthra (UiO) replacing S. Ton (AU) and H. Phan (SU).

What's next in CO$_2$PERATE?

2022 will be a year with scientific progress at its centre, with several deliverables and milestones to achieve. A significant number of secondments are planned for 2022 as well.

For events, the Annual Meeting 2021 and the Global Women's Breakfast are both held as digital event in February 2022. Physical meetings are planned for the entrepreneurship course (July) and the Annual Meeting 2022 (September).

Secondments

AU to ICIQ

STEPHANIE TON
PROJECT 9 (WP3 & 4)
SEPT.-DEC. 2021

From September to December 2021, I was lucky enough to complete my research stay with Professor Ruben Martin at the ICIQ in Tarragona, Spain. This stay was incredibly rewarding not only being able to expand the scope of the chemistry I am working with but also to experience the culture of a new country.

During my stay in Professor Martin's lab, I was able to work on two projects exploring the intricacies of nickel-catalysed reactions from a mechanistic point of view.

The first project looked at the role of electron transfer events i.e., reduction, disproportionation and comproportionation in nickel catalysis. This work was found to be particularly relevant in understanding the formation of deleterious off-cycle species relevant in carboxylation reactions.

The second project aimed to better understand the mechanism of nickel catalysed chain walking reactions through the synthesis of well-defined Ni-Alkyl complexes. Both projects were greatly aided by the state-of-the-art facilities at the ICIQ allowing me to access techniques such as EPR and Xray crystallography.

On the weekends my days were filled with exploring the beautiful town of Tarragona. I tried to take full advantage of my time in Spain enjoying many beach days, countless tapas and exploring the roman architecture of Tarragona.

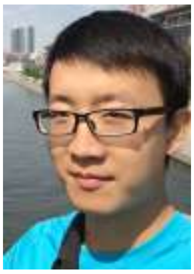
I thoroughly enjoyed my experience getting to know the group members at the ICIQ and having the chance to collaborate and learn from the other members of CO$_2$PERATE.

ICIQ building and views around Tarragona (photos: S. Ton).

Secondments

HT to AU

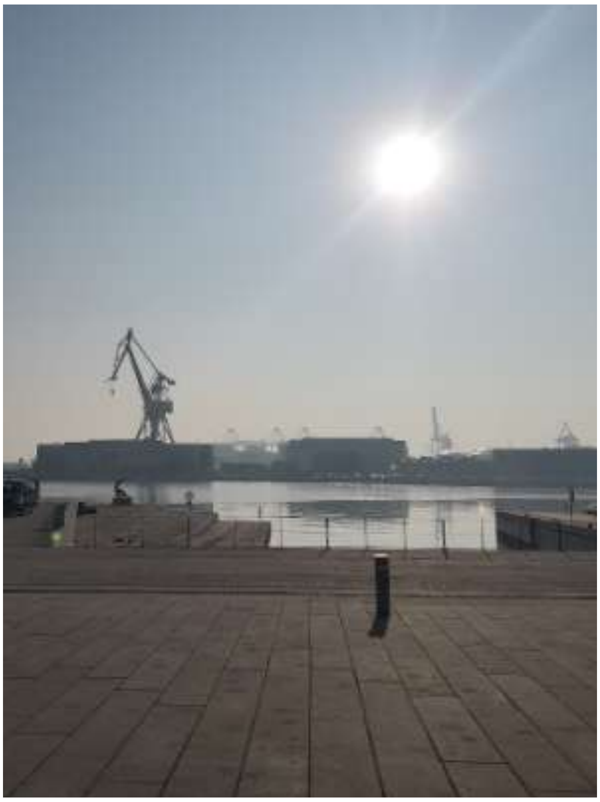
YUNFEI BAI
PROJECT 4 (WP1)
SEPT.-DEC. 2021



In 2021, from September to December, I attended a Solid-State nuclear magnetic resonance (NMR) training project at Aarhus University under the supervision of Professor Jørgen Skibsted. The NMR laboratory at Aarhus University is also known as Danish Center for Ultrahigh Field NMR Spectroscopy. It is a great pleasure to learn from the experts in the AU NMR group. It is a professional, helpful and passionate team.

Solid-State NMR is a powerful characterization method which can investigate the nucleus directly. Novel research on materials science and biology are conducted using this technique. For my secondment at Aarhus University, I have systematically learned the theoretical background, equipment operation, numerical simulation, and data analysis of the Solid-State NMR technique, and finished 11 sub-projects, including cement, zeolite, polymer, and biosolid.

A beautiful, peaceful corner of the Aarhus city centre (left) and Aarhus cathedral (right). Photos by Y. Bai..



The port of Aarhus, with view on the container terminal (photo: Y. Bai).

It is quite challenging to study the Solid-State NMR technique as a beginner, and I enjoy this experience at Aarhus University. Aarhus is a beautiful city, and I am looking forward to seeing more opportunities to collaborate with the AU NMR group!

New buildings emerging from the Aarhus coastline (photo: Y. Bai).

Secondments

EV to LIKAT

JIALI LIU
PROJECT 14 (WP1)
SEPT.-DEC. 2021

Project 14 “Theoretical studies on catalytic alkoxycarbonylation and carbonylation reactions with CO$_2$” is a part of WP1 (“Carboxylic Acids and esters from CO$_2$”).

Just two months after being a member of CO$_2$PERATE project, I had the first secondment with Prof. Matthias Beller at the LIKAT in Rostock. In this secondment, I learned so many scientific knowledge and gradually know how to cooperate with others.

The main work in LIKAT is to have an insight into experimental factors of carbonylation reactions. There are so many details, like how to stabilize the possible active species and to optimize the catalytic system. From those study, I have a whole picture about the experimental process, and this is basis for that I can propose the experimental suggestion based on the computational data.

The beautiful sunset can be admired behind the cityscape of Rostock (photo: J. Liu).

In addition, I also had a cooperative work with Sara Kopf, a PhD student of Prof. Matthias Beller. This work involves the remote deuteration of pyridine derivates and this is my first finished cooperation work. We discussed and learned a lots from her, like the different ways to measure the deuterated yield and a little knowledge about EPR.

Moreover, I learned a lot from the biweekly seminar, they present their work in a very logic way and explain so many experimental details.

In Rostock, I enjoyed the sun by the sea and going hiking on the weekend. In addition, I made lots of friends and they help me so many things. I really feel lucky to have this secondment, and which provide me this chance to learn from the other student and professor of CO_2PERATE.

The Rostock townhall during the festival of lights, held in December 2021 (photo: J. Liu).

The Dornbusch Lighthouse on Hiddensee Island, about a hundred kilometers east of Rostock (photo: J. Liu).

Early-stage researchers

Georgia Kriticou

ESR#6
UNIVERSITY OF ZÜRICH

Georgia obtained her master's degree from the University of Durham, Great Britain. In her free time, she enjoys physical activities such as hiking and swimming, as well as reading (both fiction and non-fiction!) and painting.

Why did you join CO_2PERATE?

I joined CO_2PERATE because it gives me the opportunity to work on developing new sustainable catalytic systems as well as gaining mechanistic understanding of these systems. Moreover, the use of chemical knowledge and research to solve the real-world problem of excess CO_2 in the environment is fascinating, as it shows a direct application of ESRs' progress.

Zürich from above (photo: G. Kriticou).

Finally, the planned secondments and the combination of academic and industrial research settings promote collaboration of different institutes across Europe, providing a multi-cultural network for innovation.

What is your project about?

My project revolves around the development of reliable catalytic systems for the synthesis of cyclic carbamate building blocks utilizing atmospheric CO_2 and readily available π-systems or strained systems as starting materials. Such asymmetric transformations will be achieved through electrocatalysis and the use of Ni-catalysts. The project will also involve acquiring an in-depth mechanistic understanding via kinetic studies.

The Lindt chocolate factory in Zürich (photo: G. Kriticou).

The Irchel campus (photo: G. Kriticou).

Tell us about the institution/country you are currently in.

For my PhD, I had the opportunity to move to Switzerland attending the University of Zürich, as part of the Graduate School of Chemical and Molecular Sciences Zürich.

Zürich is the largest city in Switzerland and is located in north-central Switzerland, at the north-west tip of Lake Zürich. Switzerland is the home to numerous majestic lakes, mountains and the high peaks of the Alps and is known for its ski resorts, hiking trails and chocolate.

Georgia's supervisors Cristina Nevado (UZH, main supervisor), Troels Skrydstrup (AU), and Magnus Johansson (AZ).

Early-stage researchers

Sahil Gahlawat

ESR#8
UNIVERSITY OF TROMSØ

Sahil obtained his master's degree from the Indian Institute of Technology in Roorkee, India. He enjoys yoga, cricket, and likes to follow what goes around in the world of geopolitics.

Why did you join CO$_2$PERATE?

I joined CO$_2$PERATE it is a project through which I can give my contribution towards using CO$_2$ preparing products of higher value. Carbon dioxide consumption is one the ways to reduce greenhouse gases in the atmosphere and is need of the hour.

What is your project about?

I also liked that through this project I will be able to share my ideas and interact with different research groups doing interesting work in the consortium.

CO$_2$PERATE focuses on outreach and according to me it is an important part of a PhD, and the way people are given chances to do secondments in industrial and academic nodes is very lucrative.

Sahil's supervisors Kathrin Hopmann (UiT, main supervisor), Abril Castro (UiO), and Per-Ola Norrby (AZ).

Collaborating at the Winter School 2021. From left to right: Sahil (ESR8, UiT), Sara (NordCO$_2$, HU), Ha (ESR3, SU), and Doriane (ESR7, UZH). Photo by M.-J. H. Halsør.

Tell us about the institution/country you are currently in.

I am thrilled to work in the northernmost university in the world, The Arctic University of Norway (UiT). Norway is a very beautiful country and Tromsø, where my university is located, is very appealing. The university has a good research environment with superior facilities and infrastructure. You can enjoy watching northern lights from your office room while working. There are few months during winters in which it remains dark almost all the time and, in the summers, you can enjoy the midnight sun. Especially for me, as I am from India with completely different weather patterns, these things feel like I am living the most adventurous time of my life.

Is there one thing about you that you would like others to know?

I am a technology geek and like to talk about new technological gadgets emerging in the market. This may appear as a bit boring, but believe me if you started to explore there is no out then.

Christmas decorations at the Faculty of Health Sciences, UiT (photo: M.-J. H. Halsør).

May view from the Bukta beach, on the island of Tromsø (photo: M.-J. H. Halsør).

Jiali Liu

ESR#14
EVONIK

Jiali obtained her master's degree from the Institute of Coal Chemistry at the Chinese Academy of Sciences, China. In her free time, she enjoys reading comics watching talk shows.

Why did you join CO_2PERATE?

I joined the CO_2PERATE because transforming CO_2 into high-valued carbonyl compounds is very meaningful. As well as I did theoretical work about dehydrogenation of MeOH into CO_2 using non-precious metal complex during my master. In addition, this project provides me so many opportunities to communicate and learn with other ESRs and supervisors. The most especial point for me is that I can do my research in Evonik, this will let me know the need and focus of industry. It is a so different experience for a computational chemistry student.

What is your project about?

My project focus on theoretical study of alkoxycarbonylation and carbonylation reactions using CO_2, especially catalyzed by non-precious metal complex catalyst. Our goal is to explore reaction mechanism and further improve the reaction system, even design the new catalyst with more excellent catalytic performance.

Currently, I focus on methoxycarbonylations with CO and not with CO_2 and study the substituents effect of catalyst. Because we always must start from the conventional case and model it as a benchmark.

Tell us about your institution/country you are currently in.

Evonik is one of the world's leading specialty chemicals companies, active in over 100 countries around the world with more than 36,000 employees. I work in the largest production site in Marl. I always have discussion with experimental researchers in my department and they are very nice.

I started learning the culture of Germany and taste German food, though it is so different from China. It is an interesting experience, and I can always know and try new things.

Is there one thing about you that you would like others to know?

After coming to Germany, I fell in love with döner kebab. In Germany, it usually contains seasoned sliced beef or chicken, sauce, and vegetables.

Jiali's supervisors Robert Franke (EV, main supervisor), Annette Bayer (UiT), and Troels Skrydstrup (AU).

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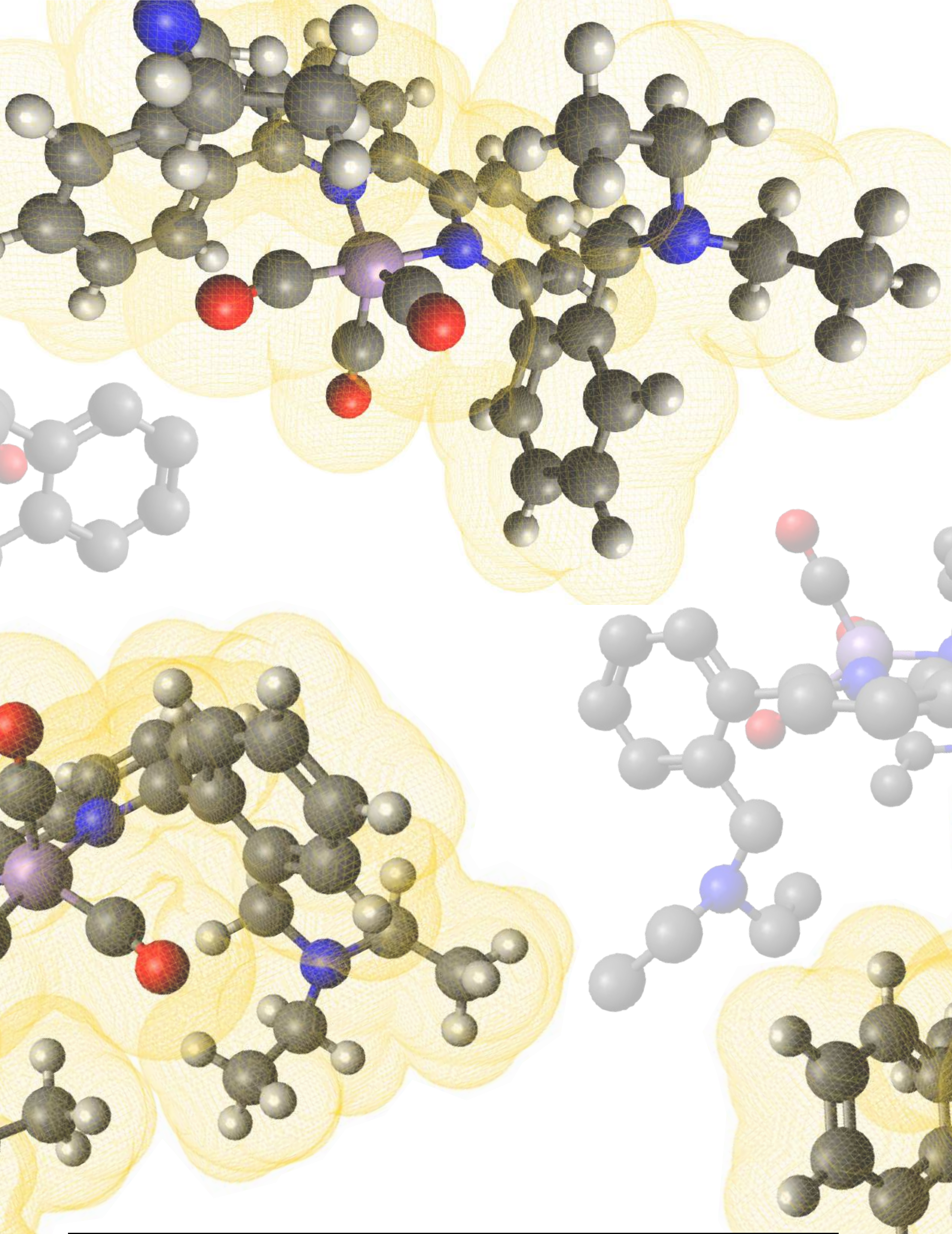

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