CH-422

Catalyst design for synthesis

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Cursus	Sem.	Type
Chimiste	MA1, MA3	Opt.

Language of teaching	English
Credits	3
Session	Winter
Semester	Fall
Exam	Written
Workload	90h
Weeks	14
Hours	**2 weekly**
Courses	2 weekly
Number of positions	

Summary

This advanced course on homogeneous catalysis explain the important role of the field in modern chemistry and provide a detailed understanding of how these catalysts work at a mechanistic level and give examples of important applications (carbon dioxid hydrogenation, hydrogen storage and delivery).

Content

- Organometallic chemistry: revision of basic ideas including structure and bonding and the implications this has on reactivity of an organic ligand coordinated to a metal centre.
- A description of the reactions involved in homogeneous catalysis, with an emphasis on the essential features required to predict which type of reactions can take place.
- Carbon dioxide hydrogenation, hydrogen storage and delivery
- Kinetics and mechanisms in formic acid dehydrogenation
- Solvent and pH in homogeneous catalysis
- General classification of different types of catalysts and their industrial relevance/importance with an emphasis on the mechanistics the following types of reactions will be studied: hydrogenation, carbon dioxide hydrogenation, carbonylation, hydroformylation, isomerisation .
- Ligand design, *i.e.* modification of ligands in order to produce more efficient and selective catalysts, will be discussed. Enantioselective ligands that give optically pure products will also be considered.
- Methods to immobilise homogeneous catalysts in alternative solvents (biphasic catalysis) will be explored with an emphasis on the strategies available and how to modify the catalyst to operate under the different conditions.
- Methods to study homogeneous catalysts *in situ*.

Keywords

homogeneous catalyst, hydrogenation, carbon dioxide hydrogenation, hydrogen storage, carbonylation, hydroformylation, isomerisation,

Learning Prerequisites

Required courses

inorganic chemisrty
organic chemistry
organometallic chemistry
kinetics
catalysis

Recommended courses

Inorganic chemistry, organic chemistry, organometallic chemistry, catalysis

Learning Outcomes

By the end of the course, the student must be able to:

- Classify catalysts and different catalysed reactions
- Explore the molecular mechanisms of catalytic processes
- Assess / Evaluate the ways that catalysts can be improved
- Design superior catalysts (in theory)

Teaching methods

Lecture course

Assessment methods

Written exam

Resources

Bibliography

Aqueous-Phase Organometallic Catalysis - Concepts and Applications, 2nd Ed, Eds. B. Cornils and W. A. Herrmann, Wiley-VCH, Weinheim, **2004**.
Catalytic Mechanisms from Spectroscopic Measurements, B. Heaton (Ed.), Wiley-VCH Verlag, Weinheim, **2005,**

Ressources en bibliothèque

- Aqueous-Phase Organometallic Catalysis / Herrmann
- Encyclopedia of Catalysis / Horváth
- Mechanisms in homogeneous catalysis / Heaton

Notes/Handbook

Encyclopedia of Catalysis, Ed. István T. Horváth, **2010**, John Wiley & Sons, Inc.,

Websites

- http://scgc.epfl.ch/telechargement_cours_chimie