Course Specifications
Valid as from the academic year 2016-2017

Organometallics and Catalysis (C002556)

Course size

<table>
<thead>
<tr>
<th>Credits</th>
<th>Study time</th>
<th>Contact hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0</td>
<td>150 h</td>
<td>45.0 h</td>
</tr>
</tbody>
</table>

Course offerings and teaching methods in academic year 2017-2018

A (semester 2)

- lecture: 30.0 h
- seminar: coached exercises 15.0 h

Lecturers in academic year 2017-2018

Van der Eycken, Johan

- WE07 lecturer-in-charge

Offered in the following programmes in 2017-2018

<table>
<thead>
<tr>
<th>Programme</th>
<th>crdts</th>
<th>offering</th>
</tr>
</thead>
<tbody>
<tr>
<td>Master of Science in Chemistry</td>
<td>6</td>
<td>A</td>
</tr>
<tr>
<td>Exchange Programme in Chemistry (master's level)</td>
<td>6</td>
<td>A</td>
</tr>
</tbody>
</table>

Teaching languages

English

Keywords

Transition metals, transition metal catalysis, ligands, oxidative addition, reductive elimination, insertion, cyclo-insertion, homogeneous catalysis, olefine metathesis

Position of the course

Basic principles of organometallic chemistry and catalysis are discussed. Emphasis is on specific properties of transition metal complexes, and their use in organic transformations which are not easy to perform using classical organic synthesis methods.

Contents

- Introduction: the 18-electron rule, types of ligands, chemical bonding model, electronic and steric effects.
- Carbonyl ligands.
- Pi-ligands: linear and cyclic.
- Other important ligands: hydrides, phosphines, complexes containing M-C, M=C and MC bonds.
- Organometallic reactions: reactions at the metal: oxidative addition, reductive elimination, ligand substitution.
- Organometallic reactions: reactions with ligand modification: insertion and retro-insertion, nucleophilic additions, electrophilic reactions.
- Homogeneous catalysis: fundamental concepts and case studies.
- Transition metal carbenes and carbynes: structure, synthesis and chemistry.
- Olefine metathesis.
- Nucleophilic addition reactions: regio- and stereoselectivity.
- Iron complexes: synthesis; nucleophilic addition to cationic and neutral complexes; mechanism of COinsertion.
- Chromium complexes: synthesis of aryl complexes; steric and electronic implications.
- Palladium complexes: synthesis of Pd(0)- and Pd(II)-complexes; nucleophilic addition to Pd(II)-complexes; cyclization reactions; Wacker oxidation process.
- Coupling reactions with palladium: with bis-hapto-1- or hapto-1/hapto-3- complexes; the Heck reaction; applications.
- Carbonylation reactions: with anionic complexes; hydroformylation with Zr- and Co-complexes; the OXO-process; decarbonylation reactions. Isomerization reactions.
- Hydrogcnation and hydroisilylation: the catalytic cycle.
- Application of carbene type complexes with Cr, Ti and Fe.
- Transition metals as protective groups.

(Aproved)
Initial competences
Have acquired extended knowledge in the field of organic and inorganic chemistry (basic as well as advanced level).

Final competences
1. Thorough insight in the methods and principles of organometallic chemistry and catalysis.
2. Thorough insight in the underlying mechanisms of organometallic chemistry and catalysis.
3. Ability to use the acquired knowledge for solving synthetic problems.
4. Ability to understand and follow new developments in the field via the literature.

Conditions for credit contract
Access to this course unit via a credit contract is determined after successful competences assessment.

Conditions for exam contract
This course unit cannot be taken via an exam contract.

Teaching methods
Lecture, seminar: coached exercises

Learning materials and price
- Copies of slides and literature references.
Cost: 0 EUR

References
"Organotransition Metal Chemistry: Applications to Organic Synthesis" (S. Davies, Pergamon Press)

Course content-related study coaching
- Classroom problem solving sessions.
- Discussion of problems is possible after each course, or upon individual appointment.

Evaluation methods
end-of-term evaluation

Examination methods in case of periodic evaluation during the first examination period
Written examination with open questions, oral examination

Examination methods in case of periodic evaluation during the second examination period
Written examination with open questions

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation
not applicable

Extra information on the examination methods
Periodic evaluation: written exam with open questions, followed by (in PE1) an oral discussion on part of the questions. The exam is application-oriented, checking acquired theoretical knowledge via exercises and problems.

Calculation of the examination mark
100% periodic evaluation

(Approved)