# 60452 - Catalysis

**Información del Plan Docente**

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| **Academic Year** | 2017/18 |
| **Faculty / School** | 100 - Facultad de Ciencias |
| **Degree** | 543 - Master's in Molecular Chemistry and Homogeneous Catalysis |
| **ECTS** | 6.0 |
| **Year** | 1 |
| **Semester** | First semester |
| **Subject Type** | Compulsory |
| **Module** | --- |

## 1.General information

## 1.1.Introduction

The course focuses on the study of the basic concepts of catalysis, the different types of catalysts, their mechanism of action and their applications. The course is divided into several different blocks: i) basic concepts in catalysis, ii) fundamentals of organometallic catalysis, iii) applications and mechanisms of organometallic catalysts, iv) principles, classification and applications of heterogeneous catalysts, and v) the design and the mechanism of action of organocatalysts. Along the course, we present a selection of some of the cutting-edge research in catalysis and their potential to meet the new challenges for sustainable development.

## 1.2.Recommendations to take this course

A mastery of the basic concepts of chemical bonding, structure and reactivity of organic and inorganic compounds is recommended. Class attendance along with continued work facilitates to pass the course.

## 1.3.Context and importance of this course in the degree

The course is part of the mandatory module entitled *Molecular Chemistry and Catalysis*. It is a mandatory subject that is taught during the first semester of the course and it has a workload of 6 ECTS credits. The course provides an advanced training for understanding the basic principles in the design of catalysts for synthetic transformations following an efficient and selective manner. Since the development and optimization of catalysts is one of the main goals of many research groups at the ISQCH, this is a fundamental subject for the realization of the *Master's Degree Final Project* in this field of research.

## 1.4.Activities and key dates

The subject of Catalysis will be taught during the first semester as well as the other compulsory subjects of this Master and the optional subjects Fundamental methodologies in synthesis and Bibliographic resources and databases. Throughout the course several control-exams and an individual or team-work will be performed. The dates of the control-exams and deadlines for the presentation of the works will be communicated well in advance.

The experimental practices of the course of *Catalysis* together with those corresponding to other subjects of the Module *Molecular Chemistry and Catalysis* constitute an integrated block. The laboratory sessions will be performed during the second half of the semester, the schedule and the laboratory will be announced well in advance.

## 2.Learning goals

### 2.1.Learning goals

The student must identify the importance of catalysis in the development of sustainable chemicals processes.

The student must know the different types of catalysts, their mode of action, advantages and disadvantages, as well as their principal applications.

The student should evaluate the activity, selectivity and environmental impact of the catalytic processes.

The student must identify key reactions in organometallic catalysis.

The student must know the main homogeneous reactions catalyzed by transition metal complexes and their reaction mechanisms.

The student should describe the different types of heterogeneous catalysts and the different strategies of immobilisation of molecular catalysts.

The student should describe the different types of organocatalyzed reactions and its applications.

The student must identify the current research lines in catalysis and its contribution to the scientific and technological development.

### 2.2.Importance of learning goals

Trained skills in this course should provide the student with an overall view of the main scientific research lines in catalysis and their importance in the development of new catalytic processes.

The design of new catalysts and the optimization of catalytic processes are key steps on the way to ensure access to affordable, reliable, sustainable and modern energy.

## 3.Aims of the course and competences

### 3.1.Aims of the course

The global objective of the course is to provide the student with an advanced training in Catalysis including the principles, mechanisms and applications of the different types of catalysts that operate both in homogeneous phase, such as organometallic catalysts and organocatalysts, and in heterogeneous phase.

### 3.2.Competences

To be able to apply newly trained skills to the study and search of new catalytic transformations.

To be able to apply concepts acquired in the field of inorganic, organic and organometallic chemistry to the design of catalysts.

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To be able to apply the fundamentals of catalysis to the synthesis of chemicals following sustainable and environmentally friendly procedures.

To identify and use the most useful literature sources in the scientific research field of catalysis.

To appreciate the potential of the catalysis to face up the new challenges for a sustainable development

To be able to communicate conclusions of a scientific research work in the field of catalysis.

## 4.Assessment (1st and 2nd call)

## 4.1.Assessment tasks (description of tasks, marking system and assessment criteria)

The evaluation of this course is based on the following activities, weighted as indicated:

1.- Control examinations of theoretical, theoretic-practical questions and problems from Module 1 and Module 2 (**P1** and **P2**). Students who get a mark equal to or higher than 5 points in both examinations will avoid these modules in the final exam.

2.- Resolution of practical exercises, theoretic-practical questions and related practical activities (**T1**).

3.- Elaboration and oral presentation of a supervised individual or team-based practical work on a scientific paper (**T2**).

4.- Global Exam: Written theoretic and problem solving test of Module 3 to be performed within the global evaluation period (**P3**). Students who had not been done the controls **P1** and **P2** or who had not get a 5 points mark, must have an additional exam with questions and problems of the corresponding modules (**P1'** y **P2'**).

The final numerical mark will be the best of the following:

Mark 1 = 0.15*(**P1** or **P1'**) + 0.25*(**P2** or **P2'**) + 0.20***P3** + 0.15* **T1** + 0.25***T2**

Mark 2 = 0.25*(**P1** or **P1'**) + 0.40*(**P2** or **P2'**) + 0.35***P3**

The rating of the students in the second annual examination session will consist in a single written exam that cover all themes of theory, problems or laboratory sessions defined as learning activities.

The number of official examination calls per registration and their use will be subjected to the statements of the *Regulation of Permanence in Master Studies* and the *Regulation of the Learning Assessment* (http://www.unizar.es/ice/images/stories/calidad/Reglamento%20Evaluacion.pdf). The latest document will also regulate the general design and scoring criteria of the assessment activities, as well as the exam schedules and timetable for the post-examination review.

## 5.Methodology, learning tasks, syllabus and resources

## 5.1.Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. A wide range of teaching and learning tasks are implemented, such as:

1. Interactive lectures (4 ECTS)

2. Seminar and problem-solving sessions (1.5 ECTS)

3. Laboratory sessions (0.5 ECTS)

## 5.2.Learning tasks

The course includes the following learning tasks:

- Interactive lectures (4 ECTS: 40 hours). In one-hour sessions, students will acquire advanced knowledge of catalysis.
- Seminar and problem-solving sessions (1.5 ECTS: 15 hours). Students will work, individually or in small groups, with several case studies and scientific papers related with the course contents.
- Tutorials. Students will own 3 hours per week for individualized tutoring.
- Laboratory sessions (0.5 ECTS: 5 hours). Attendance is compulsory. The work done in these sessions will be shared with the other courses of the *Molecular Chemistry and Catalysis* module.

## 5.3.Syllabus

The course will address the following topics:

**Section 1.**

**Basic concepts in catalysis.**

- Catalysis: general concepts. Catalysis and green chemistry. Classification of catalysts: homogeneous catalysts, heterogeneous catalysts and biocatalysts. Activity and selectivity of the catalysts. Quantification of the environmental impact. Economic importance of catalysis. Frontiers in catalysis: energy and environment.

**Fundamentals of organometallic catalysis**

- Mechanisms of organometallic catalysts. Ligands and catalyst design. Reaction mechanisms: thermodynamic and kinetic aspects. Elementary steps: substitution, oxidative addition, reductive elimination, migratory insertion, elimination and nucleophilic attack.

**Section 2**

**Organometallic catalysis in homogenous phase: applications**

- Hydrogenation and hydrogen transfer hydrogenation: mechanisms. Hydrofunctionalization reactions: hydrocyanation, hydrosilylation, hydroboration and hydroamination. Carbonylation reactions: carbonylation of methanol, carbonylation of olefins: hydroformylation, hydroaminomethylation, hydrocarboxylation and hydroesterificacion. C-C coupling reactions: alkyne functionalization and cross coupling reactions. C-H activation: mechanisms. C-H activation/functionalization reactions: oxidative coupling, hydroarylation and hydroacylation, hydrocarbon functionalization. Olefin metathesis: catalyst design and applications. Alkyne metathesis.

**Section 3**

**Organocatalysis**

- Introduction to asymmetric organocatalysis. Activation pathways in organocatalysis: covalent bond formation, hydrogen bonding, weak interactions, phase-transfer catalysts. Mechanism of action and representative examples.

**Heterogeneous Catalysis**

- Principles and concepts of heterogeneous catalysis. Classification of heterogeneous catalysts: structure and composition. Supported catalysts. Anchoring strategies: covalent and non-covalent immobilization. Non-covalent immobilization: adsorption, electrostatic interaction, hydrogen bonding, and encapsulation. Nanocatalysis. Heterogeneous catalytic processes of industrial and environmental significance.

## 5.4.Course planning and calendar

Further information concerning the timetable, classroom, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the Faculty of Science website https://ciencias.unizar.es/calendario-y-horarios, and the Master's http://masterqmch.unizar.es.

The submission of assignments will be done according to the schelude announced in advance.

The students will be provided with diverse teaching material either at reprography or through the University's virtual platform https://moodle2.unizar.es/add.

## 5.5.Bibliography and recommended resources

**BB** Berkessel, Albrecht. Asymmetric Organocatalysis: from biomimetic concepts to applications in asymmetric synthesis / Albrecht Berkessek, Harald Gröger. - 1st ed., 1st repr. Weinheim: Wiley-VCH, 2005

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**BB** Fundamentos y aplicaciones de la catálisis homogénea / editado por Luis A. Oro y Eduardo Sola. 1ª ed. Zaragoza: Luis A. Oro y Eduardo Sola, 2000

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**BB** Leeuwen, Piet W. N. M. van. Homogeneous catalysis: understanding the art / Piet W.N.M. van Leeuwen Dordrecht [etc.]: Kluwer Academic Publishers, 2004

**BB** Ross, Julian R. H. Heterogeneous catalysis: fundamentals and applications / Julian R. H. Ross Amsterdam [etc.]: Elsevier, cop. 2012 [i.e. 2011]

**BB** Rothenberg, Gadi. Catalysis: concepts and green applications / Gadi Rothenberg Weinheim: Wiley-VCH, cop. 2008

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**BC** Behr, Arno. Applied homogeneous catalysis / Arno Behr and Peter Neubert Weinheim: Wiley-VCH, cop. 2012

**BC** Hagen, Jens. Industrial catalysis: a practical approach / Jens Hagen. 2nd completely rev. and extended ed. Weinheim: Wiley-VCH, cop. 2006

**BC** Hegedus, Louis S. Transition metals in the synthesis of complex organic molecules / Louis S. Hegedus. 3rd ed. Sausalito, California: University Science Books, cop. 2010

**BC** Metal-catalysis in industrial organic processes / edited by Gian Paolo Chiusoli, Peter M. Maitlis Cambridge: Royal Society of Chemistry, cop. 2006

**BC** Pihko, P. M. Hydrogen Bonding in Organic Synthesis. Wiley-VCH, 2009

**BC** Serp, P. Nanomaterials in Catalysis. Wiley-VCH, 2013

**BC** Sheldon, Roger A. Green chemistry and catalysis / Roger Arthur Sheldon, Isabel Arends, and Ulf Hanefeld Weinheim: Wiley-VCH, cop. 2007