Universidad Zaragoza

**Academic Year/course: 2024/25**

# 27232 - Homogeneous Catalysis

## Syllabus Information

**Academic year:** 2024/25
**Subject:** 27232 - Homogeneous Catalysis
**Faculty / School:** 100 - Facultad de Ciencias
**Degree:** 452 - Degree in Chemistry
**ECTS:** 5.0
**Year:** 4
**Semester:** Second semester
**Subject type:** Optional
**Module:**

## 1. General information

The overall objective of the subject is for students to understand the mechanism of a catalytic reaction and how to use this information to design a more effective homogeneous catalyst.

Particular objectives are to study the fundamental reactions that take place in homogeneous catalysis processes catalysed by transition metal complexes and to explain the concepts of active species, catalytic precursor , reaction intermediate and transition state, relating them to the activation energy. All this will be done in the context of relevant industrial processes using homogeneous catalysts. In addition, the scientific and industrial challenges in this area of chemistry will be studied.

## 2. Learning results

In order to pass this subject, the students shall demonstrate they has acquired the following results:

1. Understand the fundamental reactions in homogeneous catalysis.

2. Know the homogeneous catalytic reactions catalysed by transition metal complexes, their reaction mechanisms and their industrial applications.

3. Choose the most suitable homogeneous catalyst for a synthetic process.

4. Propose the operative catalytic cycle in the preparation of a product.

5. Prepare, present and defend basic tutored works on homogeneous catalysis.

The knowledge acquired in the subject should provide the student with a global vision of the impact of homogeneous catalysis in the chemical industry and of the expectations it generates both in basic and applied research. The use of catalysts in homogeneous media makes possible selective chemical transformations under very mild conditions, more efficient synthesis methodologies, and the development of a chemical industry with low environmental impact.

## 3. Syllabus

**Introduction**

Basic concepts. Characteristics of homogeneous and heterogeneous catalysis. Selectivity concepts in catalytic processes . Catalysis and "green" chemistry. Coordination compounds and homogeneous catalysis. Rule of 18 electrons.

Coordinative unsaturation. Electronic and steric effects of ligands. Trans effect and influence.

**Oxidative addition and reductive elimination reactions**

Characteristics of oxidative addition reactions. Types of oxidative addition reactions. Mechanisms of the oxidative addition reactions. Oxidative addition of C-H bonds. Reductive elimination reactions.

**Insertion and elimination reactions. Attack reactions to coordinated ligands**

Insertion and elimination reactions. Mechanism of insertion reactions. Characteristics of the reactions of insertion. Alpha and beta eliminations. Modifications in the reactivity of coordinated ligands. Attack reactions to coordinated ligands.

**Isomerization**

Isomerization of alkenes: position isomerization, cis-trans isomerization, skeletal isomerization. Asymmetric isomerization: synthesis of menthol.

**Hydrogenation**

Hydrogen activation. Homogeneous hydrogenation mechanisms. Representative hydrogenation catalysts: Asymmetric hydrogenation. Non-classical mechanisms: bifunctional, ionic. Hydrogen transfer reactions.

**Carbonylation**

Carbonylation reactions. Methanol carbonylation. Carbonylation of methyl acetate. Hydroformylation.

Copolymerization of olefins and carbon monoxide.

**Oxidation of alkenes**

Oxidation reactions. The Wacker process. Epoxidation of olefins. Dihydroxylation of olefins. Oxidation of C-H bonds.

**Polymerization and oligomerization.**

Polymerization of olefins. Ziegler-Natta catalysts, metallocenes, other catalysts. Mechanism of the reactions of polymerization. Dimerization and oligomerization. SHOP process (Shell Higher Olefin Process).

**Olefin metathesis**

Metathesis reactions. Metathesis of acyclic and cyclic olefins. Mechanism of olefin metathesis reactions.

Types of metathesis catalysts. Applications of metathesis reactions.

**Hydrocyanation and hydrosilylation**

Hydrocyanation reactions.  Hydrosilylation reactions. Mechanisms of hydrosilylation reactions.

**Carbon-carbon coupling reactions**

Carbon-carbon coupling reactions: Heck's reaction. Carbon-carbon coupling reactions via transmetallation. Other coupling reactions.

## 4. Academic activities

1.- **Master classes in the classroom**: Acquisition of basic knowledge of Homogeneous Catalysis. This activity comprises 40 face-to-face hours of expository-interactive classes in large groups.

2.- **Problem solving classes and seminars**. This activity comprises 10 hours of face-to-face classes in which students, individually or in groups, will solve proposed problems and discuss topics related to the subject syllabus.

3.- **Tutoring**. Students will have 6 hours per week for individualized tutoring.

The teaching and evaluation activities will be carried out face-to-face unless, due to the health situation, the provisions issued by the competent authorities and by the University of Zaragoza make it necessary to carry them out in a telematic or semi-telematic way with rotating reduced seating capacity.

## 5. Assessment system

**Continuous Assessment**

1.- There will be two continuous evaluation tests, consisting of short answer questions and multiple choice questions. In the first test, topics 1 (Introduction) to 5 (Hydrogenation) will be evaluated and in the second test the rest of the topics will be evaluated.

To pass both tests it will be necessary to obtain a grade of 5 points out of 10 in each of them. The students who obtain a grade lower than 5, but equal or higher than 4, in one of the tests may average with the grade of another test and must achieve an average grade equal to or higher than 5. This grade is the C1 grade.

2.- In addition, there will be a problem test, which will consist of exercises similar to those proposed in the seminars. The grade for the problem test will be the C2 grade.

The grade of the subject corresponding to the continuous evaluation modality will be C3 and will be calculated as the most favourable of the following formulas:

$$C3 = C1 \times 0.85 + C2 \times 0.15$$

$$C3 = C1$$

**Overall test**

Students who have not passed the subject through continuous evaluation or who wish to improve their grade will take a global test on the dates assigned in the Faculty's exam calendar. The test will consist of short answer questions and essay type questions. A minimum grade of 5 points (out of 10) is required to pass the subject.

## 6. Sustainable Development Goals

7 - Affordable and Clean Energy
9 - Industry, Innovation and Infrastructure
12 - Responsible Production and Consumption