

60452 - Catalysis

Syllabus Information

Academic year: 2023/24

Subject: 60452 - Catalysis

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

This subject provides students with advanced training in catalysis, covering the principles, mechanisms and applications of the various types of homogeneous phase catalysts, organometallic catalysts and organocatalysts, as well as heterogeneous phase catalysts. In addition, students achieve a global vision of cutting-edge research lines in catalysis and their potential to face new challenges for sustainable development.

Sustainable Development Goals (SDGs) (<https://www.un.org/sustainabledevelopment/es/>) of the United Nations 2030 Agenda: 4: Quality Education; 7: Affordable and Clean Energy; 9: Industry, Innovation and Infrastructure; 12: Responsible Production and Consumption; and 13: Climate Action.

2. Learning results

- To identify the importance of catalysis in the development of processes and chemical products in a sustainable way.
- To know the different types of catalysts, their mode of action, advantages and disadvantages, as well as their main applications.
- To assess the activity, selectivity and environmental impact of catalytic processes.
- To identify the fundamental reactions in organometallic catalysis.
- To know the main homogeneous reactions catalysed by transition metal complexes and their mechanisms.
- To describe the different types of organocatalyzed reactions and their applications.
- To describe the different types of heterogeneous catalysts as well as the different strategies for immobilization of molecular catalysts.
- To identify current research lines in catalysis and their contribution to scientific and technological development.

3. Syllabus

Basic concepts of catalysis

Topic 1. Catalysis: general concepts.

Fundamentals of organometallic catalysis

Topic 2. Homogeneous catalysis with transition metal compounds.

Topic 3. Reaction mechanisms: thermodynamic and kinetic aspects.

Topic 4. Fundamental Processes

Organometallic catalysis in the homogeneous phase: applications

Topic 5. Hydrogenation and hydrogen transfer reactions.

Topic 6. Hydrofunctionalization reactions.

Topic 7. Carbonylation reactions.

Topic 8. Carbon-carbon coupling reactions.

Topic 9. C-H activation.

Topic 10. Olefin metathesis.

Organocatalysis

Topic 11. Activation by covalent bonds.

Topic 12. Activation by hydrogen bonding.

Supported catalysis

Topic 13. Introduction to heterogeneous catalysis

Topic 14. Supported catalysis.

4. Academic activities

Acquisition of advanced knowledge of catalysis (4 ECTS).

2. Problem solving classes and seminars (1.5 ECTS). Students, individually or in groups, will solve practical cases and work on scientific articles related to the contents of the subject.

3. Laboratory practice (0.5 ECTS). The practices of the subject together with those of other subjects of the *Molecular Chemistry and Catalysis Module* constitute an integrated block.

4. Tutorials. Students will have 6 hours per week for individualized tutoring.

5. Assessment system

1. A problem-solving exam, theoretical and/or theoretical-practical questions(**P1**) of **Topics 1-7**.

2. Solving of practical exercises, theoretical-practical questions and related practical activities(**T1**).

3. Laboratory practice(**T2**).

4. Preparation and oral presentation, individually or in groups, of a directed work based on a scientific article related to the contents of the subject(**T3**).

5. A written test within the period of global tests consisting of the solving of problems, theoretical and/or theoretical-practical questions(**P2**) corresponding to Topics 8-14. **Students** who have not taken the **P1** test or have not achieved a grade equal to or higher than 4 out of 10, must also take a test(**P1'**) consisting of the solving of problems, theoretical and/or theoretical-practical questions related to Topics 1-7.

In order to average any of the grades with the rest, it is necessary to obtain a minimum grade of 4 out of 10 in each of the two tests P1, P1' or P2 tests.

The final grade will be the best of the following grades:

$$\text{NOTE 1} = 0.30 \cdot (\mathbf{P1 \text{ or } P1'}) + 0.45 \cdot \mathbf{P2} + 0.10 \cdot \mathbf{T1} + 0.05 \cdot \mathbf{T2} + 0.10 \cdot \mathbf{T3}$$

$$\text{NOTE 2} = 0.38 \cdot (\mathbf{P1 \text{ or } P1'}) + 0.57 \cdot \mathbf{P2} + 0.05 \cdot \mathbf{T2}$$

Students will be graded in the second annual exam by means of a single written test that will include all the theory, problems and practice topics defined as programmed learning activities.