Universidad Zaragoza

Year : 2020/21

27232 - Homogeneous Catalysis

Syllabus Information

Academic Year: 2020/21
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

1.1.Aims of the course

1.2.Context and importance of this course in the degree

1.3.Recommendations to take this course

2.Learning goals

2.1.Competences

2.2.Learning goals

2.3.Importance of learning goals

3.Assessment (1st and 2nd call)

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

4.Methodology, learning tasks, syllabus and resources

4.1.Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. It favors the understanding of the different chemical processes that occur in homogeneous catalysis as well as an overview about industrial processes based on transition metal homogeneous catalysts. A wide range of teaching and learning tasks are implemented, such as lectures and tutorials.

Students are expected to participate actively in the class throughout the semester.

Classroom materials will be available via Moodle. These include a repository of the lecture notes used in class, the course syllabus, as well as other course-specific learning materials.

Further information regarding the course will be provided on the first day of class.

4.2.Learning tasks

The course includes 5 ECTS organized according to:

- Theory sessions (5 ECTS): 50 hours. lecture notes and a series of problems (and its solutions) will be available for the students. At the end of each topic, some of the problems will be solved in class by the professor and the rest will be done individually.
- Tutorials.

4.3.Syllabus

The course will address the following topics:

Section 1. Introduction

- Topic 1. Introduction to homogeneous catalysis. Basic concepts and importance of homogeneous catalysis. Green-Chemistry and catalysis. The selectivity of a catalytic process. Transition metal compounds and their application as homogeneous catalysts. The 18-electron rule. The electronic and steric effects exerted by the ligands in transition metal complexes. Coordinative unsaturation. Trans effect and trans influence.
- Topic 2. Fundamental Reactions in Homogeneous Catalysis. Oxidative addition and reductive elimination reactions Characteristics of the oxidative addition reactions. Classification of the oxidative addition reactions. Mechanisms of the oxidative addition reactions. Oxidative addition of C-H bonds to transition metal complexes. Characteristics of the reductive elimination reactions and some examples. Insertion and elimination reactions. Reactions involving attack to coordinated ligands. Characteristics of the insertion and elimination reactions. Mechanisms of the insertion reactions. Characteristics of the alpha and beta elimination reactions. Changes in the reactivity of coordinated ligands. Examples of reactions involving attack to coordinated ligands.

Section 2. Applications of the homogenous catalysis

- Topic 1. Isomerization. Isomerization of alkenes: positional isomerization, *cis-trans* isomerization, skeletal isomerization. Asymmetric Isomerization: synthesis of menthol.
- Topic 2. Hydrogenation. Hydrogen activation. Homogeneous hydrogenation mechanisms. Representative hydrogenation catalysts. Asymmetric Hydrogenation. Non-classics mechanisms: bifunctional, ionic. Hydrogen transfer reactions.
- Topic 3. Carbonylation. Characteristics of the carbonylation reactions. Carbonylation of methanol. Carbonylation of methyl acetate. Hydroformylation. Copolymerization of carbon monoxide and olefins.
- Topic 4. Oxidation. Characteristics of the oxidation reactions. The Wacker process. Epoxidation of olefins. Oxidation of C-H bonds. Polymerization and oligomerization.
- Topic 5. Olefin polymerization. Representative catalysts for olefin polymerization: Ziegler-Natta catalysts, metallocenes, other catalysts. Mechanism of polymerization reactions. Polymers and copolymers. Dimerization and oligomerization. SHOP process (Shell Higher Olefin Process).
- Topic 6. Metathesis. Metathesis reactions. Metathesis of acyclic and cyclic olefins. Mechanism of reactions of olefin metathesis. Types of metathesis catalysts. Applications of the metathesis reactions.
- Topic 7. Hydrocyanation and hydrosilylation. Characteristics of the hydrocyanation reactions. Preparation of adiponitrile by hydrocyanation of butadiene. Characteristics of the hydrosilylation reactions. Mechanisms of the hydrosilylation reactions.
- Topic 8. Carbon-carbon coupling reactions. Carbon-carbon coupling reactions: Heck reaction, carbon-carbon coupling reactions *via* transmetallation. Other C-C coupling reactions.

4.4.Course planning and calendar

Further information concerning the timetable, classroom, office hours, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the Facultad de Ciencias web (https://ciencias.unizar.es/grado-en-quimica-0).

4.5.Bibliography and recommended resources

http://biblos.unizar.es/br/br_citas.php?codigo=27232&year=2019