

## 27232 - Homogeneous Catalysis

### Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	452 - Degree in Chemistry
ECTS	5.0
Course	4
Period	Second semester
Subject Type	Optional
Module	---

### 1. Basic info

#### 1.1. Recommendations to take this course

#### 1.2. Activities and key dates for the course

### 2. Initiation

#### 2.1. Learning outcomes that define the subject

#### 2.2. Introduction

### 3. Context and competences

#### 3.1. Goals

#### 3.2. Context and meaning of the subject in the degree

#### 3.3. Competences

#### 3.4. Importance of learning outcomes

### 4. Evaluation

### 5. Activities and resources

#### 5.1. General methodological presentation

#### 5.2. Learning activities

#### 5.3. Program

#### Introduction

Basic concepts and importance of the homogeneous catalysis. Green-Chemistry and catalysis. The selectivity of the

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catalytic processes. Transition metal compounds and its application as homogeneous catalysts. The 18-electron rule. The electronic and steric effects exerted by the ligands. Coordinative unsaturation. Trans effect and trans influence.

### *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 eliminations reactions. Changes in the reactivity of coordinated ligands. Examples of reactions involving attack to coordinated ligands.

### *Applications of the homogenous catalysis*

#### **Isomerization**

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

#### **Hydrogenation**

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

#### **Carbonylation**

Characteristics of the carbonylation reactions. Carbonylation of methanol. Carbonylation of methyl acetate. Hydroformylation. Copolymerization of carbon monoxide and olefins.

#### **Oxidation**

Characteristics of the oxidation reactions. The Wacker process. Epoxidation of olefins. Oxidation of C-H bonds.

#### **Polymerization and oligomerization**

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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).

### Metathesis

Metathesis reactions. Metathesis of acyclic and cyclic olefins. Mechanism of reactions of olefin metathesis. Types of metathesis catalysts. Applications of the metathesis reactions.

### 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.

### Carbon-carbon coupling reactions

Carbon-carbon coupling reactions: Heck reaction, carbon-carbon coupling reactions *via* transmetallation. Other C-C coupling reactions.

## 5.4.Planning and scheduling

### 5.5.Bibliography and recommended resources

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- Behr, Arno. Applied homogeneous catalysis / Arno Behr and Peter Neubert Weinheim : Wiley-VCH, cop. 2012
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- Parshall, George W.. Homogeneous catalysis : the applications and chemistry of catalysis by soluble transition metal complexes / George W. Parshall, Steven D. Ittel . - 2nd ed. New York [etc.] : John Wiley & Sons, cop. 1992