27232 - Homogeneous Catalysis

Información del Plan Docente

Academic Year	2017/18
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.Introduction

1.2.Recommendations to take this course

1.3.Context and importance of this course in the degree

1.4.Activities and key dates

2.Learning goals

2.1.Learning goals

2.2.Importance of learning goals

3.Aims of the course and competences

3.1.Aims of the course

3.2.Competences

4.Assessment (1st and 2nd call)

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

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. 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 theory sessions and tutorials.

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

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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.

5.2.Learning tasks

The course includes 5 ECTS organized according to:

- Theory sessions (5 ECTS): 50 hours.

Theory sessions: 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.

5.3.Syllabus

The course will address the following topics:

Theory sessions

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

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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.

5.4.Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course please refer to the "Facultad de Ciencias" website (ciencias.unizar.es).

Universidad Zaragoza

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5.5.Bibliography and recommended resources

BB	Bhaduri, Sumit. Homogeneous catalysis : mechanisms and industrial applications / Sumit Bhaduri, Doble Mukesh New York [etc.] : Wiley-Interscience, 2000
BB	Fundamentos y aplicaciones de la catálisis homogénea / editado por Luis A. Oro y Eduardo Sola . - 2ª ed. Zaragoza : Luis A. Oro y Eduardo Sola, 2000
BB	Leeuwen, Piet W. N. M. van. Homogeneous catalysis : understanding the art / Piet W.N.M. van Leeuwen Dordrecht [etc.] : Kluwer Academic Publishers, 2004
BC	Behr, Arno. Applied homogeneous catalysis / Arno Behr and Peter Neubert Weinheim : Wiley-VCH, cop. 2012
BC	Crabtree, Robert H.. Química Organometálica de los metales de transición / Robert H. Crabtree ; Eduardo Peris Fajarnés [trad.] Castelló de la Plana : Publicacions de la Universitat Jaume I, D. L. 1997
BC	Hartwig, John F.. Organotransition metal chemistry : from bonding to catalysis / John F. Hartwig Sausalito, Ca. : University Science Books, 2010
BC	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
BC	Rothenberg, Gadi. Catalysis : concepts and green applications / Gadi Rothenberg Weinheim : Wiley-VCH, cop. 2008

LISTADO DE URLs:

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Organometallic HyperTextBook -
[http://www.ilpi.com/organomet/]