Universidad Zaragoza

Academic Year/course: 2022/23

60451 - Molecular Design in Inorganic and Organometallic Chemistry

Syllabus Information

Academic Year: 2022/23
Subject: 60451 - Molecular Design in Inorganic and Organometallic Chemistry
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

1.1. Aims of the course

This subject is one of the central topics in the framework of the *Master in Molecular Chemistry and Homogeneous Catalysis*, because provides knowledge of coordination compounds and organometallic complexes, including clusters and nanoparticles, about synthesis, bond models, properties, reactivity and current applications like the catalytic processes that are studied in another subjects as *Catalysis*, *Asymmetric Catalysis*, *Sustainable Chemistry and Catalysis* and *Supramolecular Chemistry*.

One of the main goals of the subject is that students increase their knowledge in Coordination Chemistry to be able to evaluate the effect of different complexes over some small molecules, some of which are widely used in catalytic reactions and processes. In addition, the student will realize how organic compounds change its reactivity when act as ligands bonded to the metal centers. The knowledge of the different types of M-C bond, depending on the organic groups involved, its structure and related properties will provide to the students a global perspective of the Organometallic Chemistry of the transition elements.

These approaches and objectives are aligned with the following Sustainable Development Goals (SDGs) of the United Nations 2030 Agenda (https://www.un.org/sustainabledevelopment/es/), so much so that the acquisition of this scientific knowledge will provide students with the skills required to achieve these goals, and specifically the following ones: Goal 3: Health and well-being; Goal 4: Quality education; Goal 5: Gender equality; Goal 7: Affordable and clean energy; Goal 8: Decent work and economic growth; Goal 9: Industry, innovation and infrastructure, Goal 10: Reducing inequalities, Goal 12: Responsible production and consumption, and Goal 13: Climate action .

1.2. Context and importance of this course in the degree

The subject *Molecular Design in Inorganic and Organometallic Chemistry* is included in the compulsory module of the *Master in Molecular Chemistry and Homogeneous Catalysis*. This subject is taught in the first half term of the course and it has assigned 6 ECTS credits: 4 ECTS for lectures, 1.5 ECTS for solving problems sessions with student participation, and 0.5 ECTS credits to be developed in the laboratory in coordination with other subjets of the module *Molecular Chemistry and Catalysis*. The program of the subject extend the knowledge acquired in the subjects of Inorganic Chemistry along the Degree in Chemistry and is essential for understanding the modifications in the properties and reactivity of molecules or organic fragments caused by the presence of metal, thus influencing processes of Organic Chemistry, Biochemistry and Catalysis.

1.3. Recommendations to take this course

The basic knowledge about chemical structure, bonding and reactivity of coordination and organometallic compounds is highly recommended.

Class attendance along with continued work facilitates to pass the course.

2. Learning goals

2.1. Competences

To know and predict the synthesis and stability of coordination compounds.

Capacity to recognize and make sense to the modifications suffered by the molecules coordinated to a metal center and expect its new reactivity.

Capacity to recognize the presence of metal-metal bonds in polynuclear coordination compounds or clusters.

To be able to select the method for the preparation of metal nanoparticles and for the prediction of potential applications.

To use the nomenclature and specific terminology within the framework of Inorganic Chemistry.

Capacity to recognize the different types of organometallic complexes and predict their stability.

To redict the different reactivity of organometallic complexes.

To be able to select the synthetic methods to prepare organometallic complexes of transition metals.

To be able to design and synthesize new organic, inorganic or organometallic molecules that could be of industrial and technological interest.

To be able to select and use the analytical and spectroscopic data got from standard techniques to elucidate the composition and structure of organometallic complexes.

To understand, explain and study the mechanisms of stoichiometric and catalytic reactions.

To apply methods, procedures and experimental techniques in advanced synthesis.

To know the applications of organometallic complexes in synthesis and catalysis.

To know the applications of coordination compounds and organometallic complexes in medicine.

To be able to assimilate and critically evaluate research results in Molecular Chemistry relating them with the theoretical knowledge.

2.2. Learning goals

The student must apply basic concepts of coordination chemistry to the synthesis of complexes that contain small molecules.

The student should evaluate the possible modes of coordination, bonding, properties, reactivity and potential applications.

The student must know and apply concepts of metal-metal bonding to di- or polynuclear complexes and clusters.

The student must identify the methods of synthesis, the utility and the applications of nanoparticles.

The student must know the principles and characteristics of the different M-C bonds and recognize the different families of organometallic compounds.

The student must know the usual methods in the synthesis of organometallic complexes and their general properties.

The student must predict the stability and reactivity of the different types of transition metal organometallic complexes and be able to propose methods of synthesis.

The student must be able to use the information provided from spectroscopic and analytical techniques to the characterization of the organometallic complexes.

The student must solve problems and discuss critically questions about structure and reactivity of organometallic complexes.

The student must recognize the utility of some organometallic compounds for the synthesis of organic molecules and as catalysts in chemical processes.

2.3. Importance of learning goals

The learning results of this subject are very important because they will allow the graduate to predict the stability and reactivity of different types of coordination and and organometallic compounds. Also, the learning results will allow the graduate to propose methods of synthesis and get criteria to select the appropriate information from the analytical and spectroscopic techniques for the characterization of complexes. In summary, they will provide tools to the students to develop their creative ability to perform his job as a researcher and the knowledge to predict the usefulness of inorganic and organometallic complexes in different actual aspects of Science and Technology.

3. Assessment (1st and 2nd call)

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

The evaluation of this course is based on the following activities, weighted as indicated:

1.- A mid-term examination containing theoretical, theoretic-practical questions and problems from the themes 1 to 5 of the program (**P1**).

2.- Elaboration and presentation of a supervised individual or team-based practical work on a scientific paper (**T1**).

3.- The laboratory report (**IL**) of the integrated practices carried out together with the "*Catalysis*" subject.

4.-There will be a final exam at the end of the term containing theoretical and theoretic-practical questions or problems from the themes 6 to 10 of the program (**P2**). Students who had not been done the control **P1** or who had not get a 4 points mark, must have an additional exam with questions from themes 1 to 5 (**P1'**).

In order to average the marks obtained by the student in any of the **P1**, **P1'** or **P2** tests with the rest of the marks it is essential to obtain a minimum score of 4 points out of 10.

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

NOTE 1= 0,37*(**P1** or **P1?**)+ 0,15***T1** + 0,43***P2** + 0.05***IL**

NOTE 2= 0,45***P1?** + 0,55***P2**

The rating of the students in the second annual examination session will consist in a single written exam that cover all themes of theory, problems or laboratory sessions defined as learning activities.

The number of official examination calls per registration and their use will be subjected to the statements of the *Regulation of Permanence in Master Studies* and the *Regulation of the Learning Assessment* (https://ciencias.unizar.es/normativas-asuntos-academicos). The latest document will also regulate the general design and scoring criteria of the assessment activities, as well as the exam schedules and timetable for the post-examination review.

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. A wide range of teaching and learning tasks are implemented, such as:

1. Theoretical classes.

2. Problem-solving sessions and seminars.

3. Laboratory sessions.

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

Classroom materials will be available via Moodle.

4.2. Learning tasks

The course includes the following learning tasks:

- Lectures (4 ECTS: 40 hours). Students will acquire advanced knowledge of Inorganic and Organometallic Chemistry. This activity is based on interactive teaching in the classroom in a large group.
- Seminars and problem-solving sessions (1.5 ECTS: 15 hours). Students will work, individually or in small groups, with several case studies and scientific papers related to the course contents.
- Laboratory sessions (0.5 ECTS: 5 hours). Laboratory sessions take place in the chemistry laboratory and the attendance is compulsory, as happens with the other courses of the *Chemistry and Molecular Catalysis* module.
- Guided assignments.
- Tutorial activity will be carried out mainly in remote using on-line tools. The students will have 3 hours per week for individualized tutoring.

Teaching and assessment activities will be carried out in the classroom with all students onsite unless, due to the health situation, the provisions issued by the competent authorities and the University of Zaragoza arrange to carry them out by telematics means or in a reduced rotating capacity.

4.3. Syllabus

The course will address the following topics:

Topic 1. **Fundamental concepts in Coordination Chemistry.**

- General considerations of transition metals. Structure and properties of coordination compounds. Electronic structure and bonding. Synthesis and reactivity of coordination compounds.

Topic 2. **Activation of small molecules by coordination to metal centers.**

- Coordination of CO_2 to metal centers, reactivity. Carboxylation reactions. Complexes with NO and N_2O, coordination modes of nitrogen and reduction processes. Coordination and activation of diatomic molecules. Inter - and intramolecular hydrogen bonds.

Topic 3. **Metal-metal bonds in coordination compounds.**

- Introduction and bonding types. Multiple metal-metal bond: bond order, strength and M-M distance. Preparation and reactivity of complexes with quadruple bond. Preparation and reactivity of complexes with triple bond. Complexes with quintuple bond. Other types of metal-metal bonds.

Topic 4. **Clusters Compounds.**

- Carbonyl Clusters of high and low nuclearity. The CO bond in metal carbonyls. Application of NAE and Wade rules to the structure of the clusters. Isolobular concept. Halide clusters. Synthesis of clusters and reactivity.

Topic 5. **Huge clusters and nanoparticles.**

- Classification of the nanoparticles according to the size and shape. Preparation, properties and applications of nanoparticles.

Topic 6. **Types of ligands.**

- Transition metal organometallic complexes: sigma-donor ligands. Preparation of transition-metal-alkyl and ?aryl compounds. Thermodinamic versus kinetic lability. Reactivity: Insertion reactions. Alkenyl and alkynyl complexes: synthesis, properties and applications.

Topic 7. **Transition metal complexes with M-C multiple bonds**.

- Transition metal carbene complexes. Types of carbenes: preparation, structure, binding and reactivity. Alenylidene and vinylidene complexes. Transition metal carbyne complexes: preparation, structure, bonding and reactivity. Applications.

Topic 8. **Transition metal complexes with sigma-pi M-C bonds (linear or cyclic but non aromatic ligands).**

- Synthesis, structure, bonding, reactivity and applications of complexes with olefins and conjugated di-olefins. Alkyne complexes. Allyl and enyl derivatives. Synthesis, structure, bonding and reactivity. Applications.

Topic 9. **Transition metal complexes with** sigma-pi **M-C bonds (aromatic ligands).**

- Transition metal complexes with aromatic rings. Sandwich and semisandwich complexes. Complexes with three or four membered aromatic rings. Cyclopentadienyl derivatives. Binary cyclopentadienyl complexes. Metal complexes with benzene or its derivatives as ligands. Bis(arene) metal complexes. Semisandwich arene metal carbonyls. Complexes with seven or eight membered aromatic rings. Synthesis, properties and applications.

Topic 10. Medical therapies with metal complexes.

- Essential elements. Chelation therapy. Diagnostic agents. Radiopharmaceuticals. Therapeutic agents (anticancer, antibiotic, anti-arthritis).

4.4. Course planning and calendar

Further information concerning the timetable, classroom, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the Faculty of Science website https://ciencias.unizar.es/calendario-y-horarios, and the Master's http://masterqmch.unizar.es.

The submission of assignments will be held according to the schedule that will be announced in advance.

Students will be provided with extensive scholar material either at reprography or through the University's virtual platform: https://moodle2.unizar.es/add.

The subject *Molecular Design in Inorganic and Organometallic Chemistry* will be taught in the first half term, in addition to the other 3 compulsory subjects of the Master and the optional subjects *Basic methodologies in synthesis* and *Bibliographic resources and databases.* Throughout the course some individual or team-based controls, as well as presentations of some literature works, will be carried out in order to delve into some issues. The presentation dates will be communicated in advance.

The laboratory section of the subject together with those corresponding to other subjects of the module *Molecular Chemistry and Catalysis* constitute an integrated block. Laboratory sessions will be held in the second half of the term. The dates and place will be announced well in advance.