UAB
Universitat Autònoma de Barcelona

Chemistry of Co-ordination and Organometallics

Code: 102506
ECTS Credits: 6

2024/2025

Degree	Type	Year
2502444 Chemistry	OB	3

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Teachers

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

To take Quimica de Coodinació i Organometàl·lica (Coordination and Organometallic Chemistry), it is a prerequisite to have passed the subjects Quimica dels Elements, Espectroscopia and ERCO, because those subjects will be used in the Quimica de Coodinació i Organometàl·lica course without previous explanation

Objectives and Contextualisation

Coordination and Organometallic Chemistry is a subject of the third year course of the area of knowledge of Inorganic Chemistry and its objective is to provide a broad knowledge of the Coordination Chemistry and the Organometallic Compounds of the transition metals.

Its content is mainly based on the Chemistry of the Elements of the second year, and in some of specific aspects in the subjects of second year: Espectroscopia and ERCO. On the other hand, some aspects of the Chemistry of Coordination and Organometallic are related to the Science of Materials of the third year. Upon passing this subject the student will have acquired a good part of the abilities
Basic in Inorganic Chemistry necessary for the incorporation of the labor market or for continuing its academic training.

The skills will be completed after having studied Materials Science in the second semester of the third year.

In a unified way the subject provides knowledge about the coordination compounds (chemical compounds that are the result of the interaction between a metal center that acts as Lewis acid, mainly of transition metals, and ligands that are ions or molecules, generally bases of Lewis.

The subject is structured in two parts. In the first one, the bases of the Chemistry of Coordination (ligands, binding, properties, electronic spectra and more important reactions) are studied, and in the second part the study focuses on the transition metal coordination compounds with ligands that They contain carbon as a donor atom (organometallic compounds).

The study of the organometallic compounds of the transition elements is organized by means of a presentation of the organometallic ligands, the Rule of 18 electrons, and the study of the different types of organic ligands (bond, structure and reactions) and of the most important catalytic applications of these compounds.

The subject consists of theory classes and exercises classes. The laboratory practices on Coordination andOrganometallic Chemistry are included in the Laboratori de Sintesi.

Competences

- Develop synthesis and analyses studies in chemistry from previously established procedures.
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.

Learning Outcomes

1. Analyzing the thermodynamic and kinetic factors affecting the formation of metal-carbon bond and its reactivity.
2. Apply the acquired theoretical contents to the explanation of experimental phenomena.
3. Calculate the stoichiometry of a reaction
4. Construct the major catalytic cycles involving organometallic species.
5. Critically evaluate experimental results and deduce their meaning.
6. Deduce the most likely structure of a compound using the rule of 18 electrons.
7. Deduce the stable electronic configurations of an organometallic compound.
8. Deduct the most stable of a metal ion from ligand field theory and electronic configuration Molecular Orbital in environments common coordination.
9. Deduct the splitting of the energy terms of a metal ion in an octahedral field.
10. Describe the most important reaction mechanisms.
11. Highlighting the high reactivity of the metal-carbon bond.
12. Identify the most important catalytic organometallic reactions.
13. Interpret the electronic spectra of coordination compounds.
14. Recognize the thermodynamic and kinetic parameters affecting speciation coordination and reaction mechanisms.
15. Solve problems with the help of additional bibliography provided
16. Sort and rationalize the most important reaction mechanisms of metal complexes.
17. Sort ligands within the spectrochemical series.
18. Sort organometallic compounds as the ligands present, highlighting the importance of the carbonyl ligands and phosphine.
19. Use the periodic table with ease and place each element in its correct position.

Content

Contents

Course: Third

Subject: One semester

ECTS Credits: 6 Total Hours: 6x25 = 150

Class hours: 50

Student work hours: 100

Reference book:

Shriver-Atkins, Inorganic Chemistry, 4th edition, Ed. McGraw-Hill, 2008

Consultation bibliography:

Other bibliography:

C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 2nd edition, Ed. Pearson, 2006 (chapters 19, 20, 23, 25 i 26)

D. Astruc, Organometallic Chemistry, Ed. Reverté, 2003. ISBN 978-3-540-46128-9. French ISBN 978-2-86883-493-5

J. E. Huheey, E. A. Keiter, R. L. Keiter. Inorganic Chemistry. Principles of Structure and Reactivity. Fourth Edition, Oxford University Press, 2003, Mexico

PART I. Transition metal coordination compounds

1. Generalities. (6 h = 5 T + 1P)

Definition, general properties and applications.

Coordination ligands: Structural classification. Mono and polidentate ligands. Terminal ligands, chelating and bridge ligands. Bond classification of the ligands . Stereochemistry: Coordination numbers and geometries. Constitutional and configurational isomerism. Enantiosomery in octahedral complexes.

2. Structure and linkage in the coordination compounds (I) (10 h = 7T + 3P)

Crystal Field Theory (CFT): octahedral, tetrahedral and square-planar geometries. Crystal Field stabilization energy CFSE. High and low spin complexes. Magnetic Properties, Energy of Stabilization of the Crystal Field (CFT). CFSE of octahedral complexes versus tetrahedral complexes.

Factors that influence the Crystal Field. Spectrochemical series of ligands and spectrochemical series of metals Jorgensen parameters. Distortions as a source of stabilization. Jahn-Teller effect. Distortions of octahedral geometry. Consequences of the crystalline field: ionic radii, hydration energies, oxidation states, etc. Covalence in the coordination compounds.Nephlesuetic effect Parameters by Jorgensen.

3. Structure and bonding in coordination compounds (II) (3 h = 2 T + 1P)

Theory of Molecular Orbitals (TOM) applied to the coordination compounds. Octahedral geometry Construction of the molecular orbital diagram (OM) of an octahedral complex with ligand-metal interactions. Influence of the ligand-metal interaction in the OM diagram of an octahedral complex. Justification of the series spectrochemistry

4. UV-visible spectroscopy (6 h = 4T + 2P)

Electronic spectroscopy: Introduction. Spectroscopic Terms of transition metals. Determination of the fundamental term of the free ion. Unfolding the terms in an octahedral field. Determination of the state fundamental of the complex. d-d transitions . Selection rules. Weak field approach. d^n configuration number of absorptions. Weak field equations. Orgel Diagrams. Strong field approach. Diagrams of weak-field strong correlation. Tanabe -Sugano diagrams. Interpretation of the electronic spectrum of the coordination compounds. Jahn-Teller effect. Charge-transfer transitions

5. Reactivity in the coordination compounds (3 h = 2 T + 1P)

Thermodynamic stability and formation constants. Factors that affect the thermodynamic stability of one complex Irwing-Williams Series. Hard-soft acid-bases. Chelate and macrocyclic effect. Speed law and mechanisms of reaction in the coordination compounds. Replacement reactions of ligands in octahedral and square-planar complexes. Trans effect. Electronic transfer reactions. Potential diagrams. Mechanisms of external sphere and internal sphere.

PART II. ORGANOMETALLIC COMPOUNDS OF THE ELEMENTS OF TRANSITION.

6. General aspects (3h = 2hT + 1hP)

Brief historical review. Stable electronic configurations. The rule of the 18 electrons: ionic and covalent counting. Nomenclature of organometallic compounds.

7. Types of ligands(5h = 4hT + 1hP)

Carbon monoxide Phosphines Hydrides and dihydrogen. Agostic hydrogens h^1 ligands: alkyl, alkenyl, alkynyl and aryl. h^2 ligands: alkene and alkyne. Diene an pilyene ligands not conjugated. Dinitrogen and nitrogen monoxide. Polyenyl conjugated ligands: butadiene, cyclobutadiene and cycloctatetraene. Arens. Allyl and enyl ligands. Carbenes.

8. Types of important compounds (4h = 3hT + 1hP)

Homoléptic carbonyl complexes: structure and synthesis. Reactivity of carbonyl compounds. Spectroscopy of carbonyl compounds. Metalocenes: synthesis and reactivity. Ferrocene bonding. Metalocene fluxionality. Angular metallocenes. Metallic clusters: structure and count of electrons. Synthesis of metallic clusters.

9. Reactions of organometallic compounds. (4h = 3hT + 1hP)

Lligand substitution. Oxidative addition.Reducitive elimination. Bond methasis (hydrogenolysis). Migratory insertion. 1,1 and 1,2-insertions beta elimination of hidrogen. Other eliminations of hydrogen

10. Catalysis. (6h = 5hT + 1hP)

Generalities. Reaction coordinate. Catalytic cycle Characteristics of a catalyst: activity, stability and selectivity Types of catalysis. Some examples of important catalytic processes

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
-	11	0.44	1, 2, 5, 3, 18, 16, 17, 4, 9, 6, 8, 7, 11, 13, 14, 15
-	38	1.52	1, 2, 5, 3, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
Type: Supervised			
-	4	0.16	1, 2, 5, 3, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
Type: Autonomous			

-	5	0.2	1, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
-	5	0.2	1, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
-	10	0.4	1, 2, 5, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
-	15	0.6	1, 2, 5, 3, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
-	54	2.16	1, 2, 5, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15

The student will carry out three types of activities: directed, autonomous and supervised.

1. Guided activities:

    Theoretical classes:

    Classes of problems: The knowledge acquired is applyed to solve problems and exercises related to the contents of the subject

2. Supervised activities: The student may ask the teachers of the subject supporting activities for the assimilation of the subject exposed in the theoretical and problem classes, and for the resolution of follow-up work.

3. Autonomous activities: With these activities the student alone or in a group, must achieve the competencies of the subject. In these activities, we find the study, the resolution of problems, the writing of works, the reading of texts and the search of bibliography.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
-	-	2	0.08	1, 3, 18, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14
-	-	2	0.08	1, 3, 18, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14
-	-	2	0.08	1, 2, 5, 3, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15
Global exam	85%	2	0.08	1, 3, 18, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 19, 14

Exams

For evaluation purposes, the subject is divided into two parts.

During the semester there will be two partial exams, one in each part (ExP1 and ExP2), and a global exam of recovery (ExG), all of them with a note between 0 and 10.

Homework
During the semester, a number of homework will be collected for the student's follow-up (problems resolved

individually or in group, short classroom tests, class questions, etc.). Each student will obtain, therefore, two Homework notes (S1 and S2), which will be the weighted averages of the grades obtained in the Homework tests for each part of the subject.

Qualifications:
Each part of the subject will have a qualification (Not1 and Not2) that will be:
Not1 = 0.85 x ExP1 + 0.15 x S1
Not2 = 0.85 x ExP2 + 0.15 x S2
The final grade (NF) will be obtained as follows:
NF = (Not1 + Not2) / 2

To pass the subject per course, the following two conditions must be fulfilled:
1) The final grade of the subject (NF) must be ≥ 5.0
2) To be able to make average, ExP1 and ExP2 must be ≥ 4.5

If any of the previous requirements are not met, the student must take the final exam, where they can choose to make one or both partials, since the subjects of each partial will be separated and identified as such (NotR1 and NotR2). The NFR will be calculated by replacing the ExP1 and/or ExP2 values with those obtained in the ExR1 and/or ExR2 final test.

To participate in the final exam, students must have been previously evaluated in a set of activities whose weight is equivalent to a minimum of two thirds of the total grade for the subject.

To pass the subject in the final exam, the following two conditions must be met:

1) The final course grade (NFR) must be ≥ 5.0

2) For averaging, ExR1 and ExR2 must be ≥ 4.5

The final mark in the global exam is calculated:

NFR = (NotR1 + NotR2)/2

NotR1 = 0.85 x ExR1 +0.15xS1

NotR2 = 0.85 x ExR2 + 0.15 x S2

Students who do not pass the subject because they do not improve one of the bloks, regardless of which one is your overall average will get a maximum final grade of 4.5.

The students who pass the course by partial examinations but want to improve their qualification, may submit to the global two part test.
The Recovery examination note will replace the note that could be obtained from the sets of the two partials and, for So much, we will have a weight of 85% (the mark of the homework can not be recovered).
To the global examination, the student will not opt for the qualification of matrícula d'honor

The final grades of the approved students can be normalized from 0 to 10 (the maximum grade must be 10, all respecting the order, and the note may be increased up to 1.5 points) in order to achieve the distribution between Aprovat, Notable, Excellent, and MH.

If the student has been evaluated in a maximum of 33% of the assessments and gives up the subject, the final grade will be NOT EVALUABLE.

Single assessment:
Students who have taken the single assessment mode will have to take a final test consisting of an exam on the whole subject to be taken on the day on which the students of the continuous assessment take the exam of the second midterm. The student's grade will be the mark obtained in this test.
If the final mark does not reach 5, the student has another opportunity to pass the course by means of the make-up exam that will be held on the date set by the degree coordination office. The student's grade will be the mark obtained in this exam.

A student is graded as "*non-assessable*" following the same criterion as for the continuous evaluation.

Students must act honestly throughout the course. The dishonest attitudes (cheat, copy or any action aimed at distorting an evaluation) in any homework or examination test will Suspès, rating with a final grade of 0 in the subject, regardless of the other notes obtained by the student.

In particular, during written tests,mobile phonesor any other telecommunication device must be disconnected and kept in bags or backpacks, other communication device must be disconnected and stored in bags or backpacks that they must be on the platform. In case it is detected that a student carries some unauthorized device during the exam and , the student will be expelled from the classroom and will have a qualification of "suspès" to the subject.

Bibliography

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Software

If case the lectures are online: Teams

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	first semester	morning-mixed
(PAUL) Classroom practices	2	Catalan	first semester	afternoon
(TE) Theory	1	Catalan	first semester	morning-mixed
(TE) Theory	2	Catalan	first semester	afternoon