

**Chemistry of Co-ordination and Organometallics**

Code: 102506  
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	3	1

### Contact

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### Use of Languages

Principal working language: catalan (cat)  
Some groups entirely in English: No  
Some groups entirely in Catalan: Yes  
Some groups entirely in Spanish: No

### Teachers

Josefina Pons Picart  
Juli Real Obradors  
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### Prerequisites

To take Química de Coordinació i Organometàl·lica (Coordination and Organometallic Chemistry), it is a prerequisite to have passed the subjects Química dels Elements, Espectroscòpia and ERCO, because those subjects will be used in the Química de Coordinació 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: Espectroscòpia 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 and Organometallic 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. Nephelauctic 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 ( $3h = 2T + 1P$ )

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 and p-lyene ligands not conjugated. Dinitrogen and nitrogen monoxide. Polyenyl conjugated ligands: butadiene, cyclobutadiene and cyclooctatetraene. Arenes. Allyl and enyl ligands. Carbenes.

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

Homoleptic carbonyl complexes: structure and synthesis. Reactivity of carbonyl compounds. Spectroscopy of carbonyl compounds. Metallocenes: synthesis and reactivity. Ferrocene bonding. Metallocene fluxionality. Angular metallocenes. Metallic clusters: structure and count of electrons. Synthesis of metallic clusters.

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

Ligand substitution. Oxidative addition. Reductive elimination. Bond metathesis (hydrogenolysis). Migratory insertion. 1,1 and 1,2-insertions beta elimination of hydrogen. 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

## Methodology

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

#### 1. Guided activities: Attendance is compulsory and carried out in the presence of a teacher.

Theoretical classes: The teacher exposes the contents of the subject and answer to the possible doubts that the student could be ask.

Classes of problems: The knowledge acquired in the lectureclasses and in the autonomous activities of the student, mainly through the study, apply to solving 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.

## Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
-	13	0.52	1, 2, 5, 3, 18, 16, 17, 4, 9, 6, 8, 7, 11, 13, 14, 15
-	37	1.48	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
-	53	2.12	1, 2, 5, 18, 16, 17, 4, 9, 6, 8, 7, 10, 11, 12, 13, 14, 15

## Assessment

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### 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:

$$\text{Not1} = 0.85 \times \text{ExP1} + 0.15 \times \text{S1}$$

$$\text{Not2} = 0.85 \times \text{ExP2} + 0.15 \times \text{S2}$$

The final grade (NF) will be obtained as follows:

$$\text{NF} = (\text{Not1} + \text{Not2}) / 2$$

To pass the subject per course, the following two conditions must be fulfilled:

- 1) The final grade of the subject (NF) must be  $\geq 5.0$
- 2) To be able to make average, ExP1 and ExP2 must be  $\geq 4.0$

If the previous requirement is not met, the student must submit to a global examination, where one or both partial can be recovered, since the subjects of each partial will be separated and identified as such (NR1 and NR2). The NF will be calculated by replacing the values of Not1 and / or Not2 for those obtained in the NR1 and / or NR2 recovery test.

To participate in the recovery examination students must have previously been evaluated in a set of activities the weight of which is equivalent to a minimum of two thirds of the total grade of the subject.

To pass the subject of the global exam the following two conditions must be met:

- 1) The final grade of the subject must be  $\geq 5.0$
- 2) To be able to make average, Not1 and Not2 (NR1 and NR2 in case of recovery) must be  $\geq 4.0$

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.

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 phones or 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.

## 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

## Bibliography

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