



## COURSE DATA

## Data Subject

Code	34200
Name	Inorganic Chemistry III
Cycle	Grade
ECTS Credits	6.0
Academic year	2023 - 2024

## Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	3	First term
1929 - D.D. in Physics-Chemistry	Double Degree Program Physics and Chemistry	4	First term

## Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	8 - Inorganic Chemistry	Obligatory
1929 - D.D. in Physics-Chemistry	4 - Cuarto Curso (Obligatorio)	Obligatory

## Coordination

Name	Department
GARCIA-ESPAÑA MONSONIS, ENRIQUE	320 - Inorganic Chemistry

## SUMMARY

The compulsory subject Inorganic Chemistry III of 6 credits is included in the field Inorganic Chemistry of the fundamental chemistry module and is taught in the sixth semester of the degree in Chemistry

After the study of Inorganic Chemistry I and II, where they have acquired the basic knowledge of the subject matter and we have studied the properties of chemical elements and their compounds, inorganic chemistry III focuses on the study of the coordination and organometallic compounds.

The coordination and organometallic compounds play an important role in Inorganic Chemistry and represent a way of approaching the study of this subject matter applicable to a wide variety of systems. Its study has an integrator character, it brings together concepts and theories with experimental facts and covers from the electronic structure and molecular synthesis and reactivity of the substances, thermodynamics and kinetics, basic studies and applications. By its nature, extends from the theoretical chemistry to Biochemistry and organometallic chemistry are blurring the boundaries between the conventional Inorganic Chemistry and Organic Chemistry. The subject Coordination Chemistry, 6 credits,



and Organometallic Chemistry, 4.5 credits, will complete these topics. Currently, the area of new materials is progressing very quickly and there is a marked interest in the synthesis and properties of new inorganic solids. The items included in the subject Inorganic Chemistry III that will enable the student to understand basic concepts of solids and will complemented with the compulsory subject Science of Materials, 6 credits.

The subject Inorganic Chemistry III contains a theme of symmetry and group theory, useful tool in chemistry, which is needed to address with rigor, some aspects of the coordination compounds of transition metals.

## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

**1108 - Degree in Chemistry V1-2009 :**

**1110 - Degree in Chemistry V2-2018 :**

**1929 - Double Degree in Physics and Chemistry :**

**1934 - Programa de doble Grado Química-Ingeniería Química\_2023 :**

### R4-OBLIGATION TO HAVE SUCCESSFULLY COMPLETED THE COURSE

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

### Other requirements

Students should have completed and passed the subjects I Inorganic Chemistry and Inorganic Chemistry II.

## OUTCOMES

### 1110 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.



- Show inductive and deductive reasoning ability.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications.
- Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.
- Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Develop sustainable and environmentally friendly methods.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.



- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

## LEARNING OUTCOMES

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Inorganic Chemistry III that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Inorganic Chemistry III related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	<b>Competences of the subject Inorganic Chemistry III that contemplate the learning outcomes EUROBACHELOR®</b>
Major aspects of chemical terminology, nomenclature, conventions and units.	Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units..(CE1)
The major types of chemical reaction and the main characteristics associated with them.	Demonstrate knowledge of the main types of chemical reaction and their main characteristics.(CE4)



The principal techniques of structural investigations, including spectroscopy	Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7).
	Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes..(CE12).
	Handle the instrumentation used in the different areas of chemistry..(CE19).
	Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds..(CE8)
The principles of thermodynamics and their applications to chemistry	Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry..(CE6).
The principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules	Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules..(CE5).
The kinetics of chemical change, including catalysis; the mechanistic interpretation of chemical reactions	Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry..(CE6).
The structural features of chemical elements and their compounds, including stereochemistry.	Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7).
	Relate the macroscopic properties and the properties of individual atoms and





	molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.(CE11).
	Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes..(CE12).
The structure and reactivity of important classes o  biomolecules and the chemistry of important biological processes	Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes..(CE12).
	Relate chemistry with other disciplines.(CE26).

## COMPETENCES AND COGNITIVE SKILLS

The learning process should allow the degree graduates to demonstrate:

	<b>Competences of the subject Inorganic Chemistry III that contemplate the learning outcomes EUROBACHELOR®</b>
Ability to demonstrate knowledge and understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14).
	Recognise and analyse new problems and plan strategies to solve them..(CE15).



	Understand the qualitative and quantitative aspects of chemical problems..(CE24).
<b>GENERAL COMPETENCES</b>	
<b>The learning process should allow the degree graduates to demonstrate:</b>	
	<b>Competences of the subject Inorganic Chemistry III that contemplate the learning outcomes EUROBACHELOR®</b>
Ability to apply practical knowledge to solve problems related to qualitative and quantitative information.	Solve problems effectively..(CG4).
	Solve qualitative and quantitative problems following previously developed models..(CE14).
	Relate theory and experimentation..(CE22).
	Recognise and evaluate chemical processes in daily life..(CE23).
	Understand the qualitative and quantitative aspects of chemical problems..(CE24).

## DESCRIPTION OF CONTENTS

### 1. Molecular symmetry

- 1.1 Symmetry elements and operations.
- 1.2. Point groups of symmetry. Determination of the point group symmetry of a molecule.  $C_{4v}$ ,  $D_{3h}$ ,  $D_{4h}$   $T_d$  and  $O$  point groups.
- 1.4 Character tables. Species of symmetry. Symmetry of atomic orbitals.
- 1.4.-Application of symmetry. Chirality, molecular vibrations. IR and RAMAN spectra:  $H_2O$  molecule, stretching vibrations of carbonyl groups in metal carbonyls. Determination of group orbitals in octahedral complexes.



## **2. Coordination and Organometallic transition metal compounds**

- 2.1.- Historical aspects: Alfred Wërner and his time. Definition of coordination compound.
- 2.2.- General characteristics: oxidation state. Index and coordination geometry. Square, tetrahedral and octahedral complexes. Geometry and coordination symmetry. Idealization of coordination symmetry.
- 2.3.- Types of ligands. Classification: nature of the donor atom, denticity, nature of the metal-ligand bond, ligands in organometallic chemistry.
- 2.4.- Isomery in coordination compounds

## **3. The bond nature and electronic structure**

- 3.1- Introduction. Valence bond theory: high and low spin complexes.
- 3.2.- Crystal field theory. Factors that affect the crystalline field stabilization energy. Octahedral complexes, weak and strong field complexes. Tetrahedral complexes. Jahn-Teller effect. Square complexes
- 3.3.- Molecular orbital theory. Diagram of molecular orbitals and electronic configuration of octahedral, tetrahedral, square complexes. Angular overlap model. Energy splitting diagrams of d orbitals in complexes of other symmetries.
- 3.4.- Terms and energy levels. d-d Transitions in coordination compounds. Tanabe-Sugano diagrams.

## **4. Reactions of the metal complexes: Thermodynamic and kinetic aspects of the coordination compounds.**

- 4.1. Stability of coordination compounds. Stability constants: global and successive constants. Determination of stability constants. Stability correlations Statistical effect. Chelate effect. Macrocyclic effect. Cryptate effect. Selectivity.
- 4.2.- Reactions and mechanisms in coordination chemistry. Introduction. Ligand substitution reactions. Metal ions in aqueous solution; water exchange reactions: labile and inert metal complexes. Mechanisms of ligand substitution reactions: dissociation, exchange and association. Reactions of ligand substitution in octahedral complexes. Experimental evidence for dissociative mechanisms in octahedral complexes. Associative mechanisms in octahedral complexes. The conjugate base mechanism. Kinetic aspects of the chelate effect. Stereochemistry of the reactions. Reactions of ligand substitution in square complexes. Trans effect. Redox reactions: mechanisms of external sphere and internal sphere.
- 4.3.- Reactions in organometallic chemistry and catalysis. Types of reactions: Dissociation reactions and ligand substitution. Reactions of oxidative addition and reductive elimination. Insertion reactions. Hydride elimination reactions. Cyclometalation Principles of catalysis. Examples of catalytic processes in the chemical industry.





## WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Study and independent work	70,00	0
Preparation of evaluation activities	20,00	0
<b>TOTAL</b>	<b>150,00</b>	

## TEACHING METHODOLOGY

The subject is raised so that the student is the protagonist of their own learning and vertebrará around four axes:

**Participatory lectures**-in those classes the teacher give an overview of the topic object of study with special emphasis on the key concepts or of particular complexity. Indicate those most recommended resources that complement the topic on personal study time. The teacher will induce the student to participate in the discussions that arise through exposure of the subject.

**Practical classes and seminars**-these classes are carried out the specific application of the knowledge that students have acquired in theory classes. Students must previously have worked the problems will be resolved. The resolution of these problems is carried out on some occasions by the teacher and in another case by the students well in group, either on an individual basis.

**Tutoring**-students attend them in groups and will be one hour. In them, teacher will guide the student on the elements that make up the learning process, at the same time which will evaluate their process of learning in a global way. The student will receive a list of questions and problems that you will exercise on each of the aspects dealt with in class sessions. Also, tutorials will serve to resolve all questions that have been able to arise during classes and guide students on the methods of work more useful to the resolution of problems that may arise.

**Seminars and Conference:** Seminars and Conference will focus on complementary aspects of their training in Inorganic Chemistry. For this task, students attending the event and answer a questionnaire prepared by the instructor.

## EVALUATION

### FIRST CALL

**Modality A**

The knowledge acquired will be evaluated through a final test on the date established by the Faculty and will account for 70% of the final score. The exam will consist of objective questions about the knowledge that is considered basic (see the list of learning outcomes) as well as of numerical exercises necessary to evaluate the aspects of the subject that appear in the different topics.

A 30% of the final score will be attributed to the student's participation in any of the activities proposed along the course related to the subject, among which it is worth highlighting:

- Presentation of problems and exercises.
- Attendance and participation in the discussions.
- Resolution of problems and raising doubts.
- Realization of works and/or oral presentations.
- Realization of written tests.
- Any other complementary training activity determined by the teacher. The final mark will be that of the final test plus the one obtained in all the activities that are proposed, with the percentages indicated for each one of them. To pass the subject, the student must obtain a minimum grade of 4.5 in the final test and the weighted average must be equal to or greater than 5.

**Modality B**

The student who, for justified reasons, cannot attend class regularly can take advantage, within a maximum period of one month from the beginning of the course, to be evaluated solely by means of a written exam on the date set by the Faculty, and the final grade of the student will be the exam.

To pass the subject, the student must obtain a grade equal to or greater than 5 in this exam.

**SECOND CALL**

In the second call, the marks obtained in the activities proposed during the course (continuous assessment) can be maintained, if the student agrees, with the same conditions and percentages described for the first call. The written exam of the second call will be held on the date set by the Faculty.

**Final warning**

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), *"it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents"*.



## REFERENCES

### Basic

- Housecroft, C. E.; Sharpe, A. G.; Inorganic Chemistry, ed. Pearson Prentice-Hall, 3<sup>a</sup> edició, 2008. ISBN: 978-0-13-175553-6.  
(En format separat, s'ha publicat el manual de respostes als exercicis plantejats. Existeix una traducció a l'espanyol de la 2<sup>a</sup> edició i del manual de respostes d'Ed. Pearson Prentice-Hall, 2006.)
- Atkins, P. W.; Overton, T. L.; Rourke, J. P.; Weller, M. T. y Armstrong, F. A.; Shriver & Atkins: Inorganic Chemistry, ed. Oxford, 5<sup>a</sup> edició, 2010. ISBN: 978-0-19-923617-6.  
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- Rayner-Canham, G.; Overton, T.; Descriptive Inorganic Chemistry y Student solutions manual for descriptive inorganic chemistry, ed. W. H. Freeman, 4<sup>a</sup> edició, 2006. ISBN 10: 1-4292-1814-2.  
(Existeix una traducció al castellà de la 2<sup>a</sup> edició de G. Rayner-Canham, Química Inorgánica Descriptiva, ed. Prentice Hall, 2000)
- Miessler, G. L.; Tarr, D. A., Inorganic Chemistry, 4<sup>a</sup> edició, ed. Pearson/Prentice Hall, 2011. ISBN-13: 978-0136128663
- Smart, L., Moore, E., Química del estado sólido. Una introducción. Addison-Wesley Iberoamericana, Wilmington, 1995.
- J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic chemistry: principles of structure and reactivity, 4th ed

### Additional

- Cotton, F. A.; Wilkinson, G.; Murillo, C. A.; Bochmann, M.; Advanced Inorganic Chemistry, ed. Wiley-Interscience, 6<sup>a</sup> edició, 1999. ISBN: 978-0-471-19957-1  
Existeix una traducció al castellà de la 4<sup>a</sup> edició, F. A. Cotton y G. Wilkinson, Química Inorgánica Avanzada, ed. Limusa, 1987.
- Greenwood, N. N.; Earnshaw, A.; Chemistry of the Elements, ed. Elsevier Science, 2<sup>a</sup> edició, 1997 (corregida en 1998, con reimpresiones en 2001 y 2002). ISBN: 0-7506-3365-4.
- Purcell, K. F.; Kotz, J. C.; Inorganic Chemistry, Saunders, 1977 (existe traducció al castellà, editorial Reverté).