

**COURSE DATA****Data Subject**

<b>Code</b>	44605
<b>Name</b>	Advanced inorganic chemistry
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	5.0
<b>Academic year</b>	2018 - 2019

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2218 - M.U. en Química	Faculty of Chemistry	1	First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2218 - M.U. en Química	1 - Advanced chemistry	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
UBEDA PICOT, M ANGELES	320 - Inorganic Chemistry

**SUMMARY**

The subject Advanced Inorganic Chemistry (5 credits) is part of the Advanced Chemistry subject area and is taught in the first semester of the Master's Degree in Chemistry of the University of Valencia. It aims to expand and supplement the knowledge on inorganic chemistry acquired in the Degree in Chemistry. Specifically, the course will provide in-depth knowledge of organometallic chemistry, bioinorganic chemistry, supramolecular chemistry and coordination polymers.

The section on organometallic chemistry will cover the synthesis, characterisation and reactivity of organometallic compounds and their importance as catalysts in industrial processes and in organic synthesis. In bioinorganic chemistry, the presence of metallic elements in living organisms will be studied, as well as their interaction with biological ligands, the properties that they are able to develop (catalysis, electron transfer, structural properties, etc.) and the most recent advances in inorganic medicinal chemistry. In supramolecular chemistry, we will review the basics of molecular recognition of both metal ions and other chemical species such as anions of environmental interest or of biological relevance. The transport of inorganic species through membranes and supramolecular catalysis will also be considered. Finally, examples of sensors and/or elemental molecular machines will be presented. The units on coordination polymers are intended to provide the basic tools for the description and design of coordination networks, for the discussion of phenomenologies in interpenetrating networks and flexibility, and for the presentation of the different types of bridging ligands, their forms of coordination



and their appropriate metal centres. An important aspect of this section will be the discussion of the properties derived from these networks (magnetism, porosity, chirality, catalysis, luminescence, etc.).

## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

### Other requirements

Prior knowledge of chemistry is required, at the level taught in the qualifications listed in the recommended profile for admission of candidates to the Masters Degree.

## OUTCOMES

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- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Promote, in academic and professional contexts in the field of economic policy, ... technological, social or cultural progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) the principles of equal opportunities and universal accessibility for people with disabilities and c) the values of a culture of peace and of democratic values.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.

## LEARNING OUTCOMES



At the end of the teaching-learning process, the student should be able to:

- Organometallic chemistry
  - Know the different types of organometallic compounds and predict their stability and synthesis methods.
  - Characterise these compounds structurally and study in detail their different types of characteristic reactivity.
  - Study major catalytic processes in which such compounds are involved as catalysts, both in industry and in organic synthesis.
- Bioinorganic chemistry
  - Identify the elements present in living systems, emphasizing the role of the metal ions that interact with biological ligands and their specific coordination mode, which is more complex than that observed for simple compounds.
  - Explain how metal ions are selected by organisms taking into account their final functions.
  - Understand the properties derived from the interaction of metal ions with biological ligands, such as electron transfer, catalysis, signalling, regulation and properties of structural nature.
  - Be up-to-dated with the frontiers of knowledge in the field of bioinorganic chemistry.
- Supramolecular chemistry
  - Know the basic aspects of molecular recognition of spherical cations, transition metals, anionic species and neutral molecules.
  - Analyse the thermodynamic and kinetic nature of molecular recognition processes.
  - Sort transport processes and, in particular, analyse those mediated by ionophores.
  - Know examples of molecular catalysis, both dependent and independent of metal centres.
  - Understand the basics of sensors and molecular machines.
- Coordination polymers
  - Identify different types of coordinating networks and their intrinsic properties such as rigidity, malleability, interpenetration and porosity.
  - Analyse the different types of porous coordination polymers based on their construction units (types of bridge ligands, nature of the metals involved).
  - Know the physicochemical properties of porous coordination polymers (magnetic, chiral, reactive, selectivity, etc.)

## DESCRIPTION OF CONTENTS



## 1. Organometallic chemistry

Descriptive by type of ligand

- Introduction. Preparation, structure and bonding.
- Compounds containing  $\pi$ -donor ligands. Compounds with  $\sigma$ -donor ligands.
- Activation of small molecules. Compounds with phosphorus-donor ligands.

Reactivity

- Substitution reactions. Oxidative addition reactions. Reductive elimination reactions.
- Insertion and removal reactions. Electrophilic and nucleophilic addition and abstraction reactions on coordinated ligands.

Catalysis

- Reactions with olefins and other unsaturated compounds.
- Major industrial processes with homogeneous catalysts.
- Coupling reactions. Other catalytic processes.

## 2. Bioinorganic chemistry

- Introduction. Essential and trace elements. Terminology. Techniques in bioinorganic chemistry.
- Storage and transport of metals. Siderophores, transferrin and ferritin.
- Transport of  $O_2$ . Myoglobin, hemoglobin, mechanisms.
- Electron transfer processes. Cytochromes, FeS clusters, blue copper proteins.
- Catalytic processes. Acid-base catalysis (zinc, iron and magnesium enzymes);  $O_2$  and  $H_2O_2$  reduction (peroxidases, oxidases and oxygenases); catalytic processes of cobalt-containing enzymes.
- Gene transcription. Zinc fingers.
- Biological cycles.  $N_2$  and  $H_2$  cycles.
- Chemistry of the elements in medicine. Chelation therapy, cancer treatment, anti-arthritic agents, image diagnosis.

## 3. Supramolecular chemistry

- Molecular recognition. Spherical cations. Transition metals. Anionic and neutral species. Thermodynamic and kinetic aspects of molecular recognition.
- Transport processes in supramolecular chemistry. Bipod transport processes: active and passive transport. Cation transport. Anion transport. Coupled transport processes. Coupled transport processes. Photon-coupled transport processes.
- Supramolecular catalysis. Metal-independent catalysis. Metal-dependent catalysis. Nucleotide and oligonucleotide activation.
- Supramolecular devices. Semiochemistry. Supramolecular photochemistry. Rotaxanes and catenanes.





#### 4. Coordination polymers

- Introduction. Crystal engineering; metalosupramolecules; coordination polymers; synthetic methods.
- Networks, a description and design tool. Network definition; networks identification; one-dimensional (1D) and two-dimensional networks (2D); common three-dimensional networks (3D).
- Interpenetration. Nomenclature; interpenetration in 1D, 2D and 3D networks; interpretation of networks with different composition, topology and dimensions; self-penetration.
- Flexibility in coordination polymers. Introduction; supramolecular isomerism; flexibility of the structural units; synthetic approach; effect of solvent and other guest molecules; counterions; weak interactions.
- Transition metal coordination polymers. Types of bridging ligands; pseudohalides; anionic nitriles; pyridine-group derivative ligands; 5-membered rings nitrogen-givers derivative ligands; ligands with carboxylate groups; other bridging ligands.
- Properties. Porosity; chirality; reactivity; luminescence; conductivity; magnetism.

#### WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	35,00	100
Tutorials	5,00	100
Seminars	5,00	100
Computer classroom practice	5,00	100
Development of individual work	15,00	0
Study and independent work	30,00	0
Readings supplementary material	10,00	0
Preparation of evaluation activities	20,00	0
<b>TOTAL</b>	<b>125,00</b>	

#### TEACHING METHODOLOGY

- **Participative theoretical lectures.** The lecturer will provide an overview of the subject under study, placing particular emphasis on key or especially complex concepts and will advise on the most appropriate resources to complement the topic. In addition, students will be encouraged to participate in the discussions that may arise during lectures.
- **Seminars.** These sessions will be aimed at the implementation of the knowledge acquired by students in lectures, by analysing scientific articles on specific aspects of the subject, resolution of issues, etc.
- **Virtual classroom.** In this space, both the lecturer and the students will upload material related with the development of the different thematic units (texts, exercises, articles, etc.).



## EVALUATION

The final mark of the course, for both the first and second examination sitting, will be obtained from:

- **Written tests:** At the end of each of the four sections that constitute the subject Advanced Inorganic Chemistry, there will be a written test based on the course learning outcomes and specific objectives. To pass, students must obtain a minimum score of 5 in each of the tests. These results will account for 80% of the assessment.

- **The preparation and oral presentation** made by the students of assignments on **topics put forward** by the lecturer at the end of each unit will account for 20% of the assessment.

The mark required to pass is 5.

## REFERENCES

### Basic

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- W. Kaim, B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life. An Introduction and Guide. Ed. Wiley, 2013.
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- M. Vallet, J. Faus, E. García-España, J. Moratal. Introducción a la Química Bioinorgánica. Ed. Síntesis, 2003.
- J.W. Steed and J. L. Atwood. Supramolecular Chemistry. John Wiley and sons, (New York) 2000.
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