COURSE DATA

Data Subject	
Code	44605
Name	Advanced inorganic chemistry
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

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

Subject-matter

Degree	Subject-matter	Character
2218 - M.U. en Química	1 - Advanced chemistry	Obligatory

Coordination

Name	Department
REAL CABEZOS, JOSE ANTONIO	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.). 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:

- **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.

- **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.).

- **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.

- **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.

DESCRIPTION OF CONTENTS

1. Bioinorganic chemistry

-Introduction. Essential and trace elements. Terminology. Techniques in bioinorganic chemistry.
-Storage and transport of metals. Siderophores, transferrin and ferritin.
-Transport of O2. Myoglobin, hemoglobin, mechanisms.
-Electron transfer processes. Cytochromes, FeS clusters, blue copper proteins.
-Nitric oxide: chemical and biological properties. Introduction.
-Electronic structure of NO. Basic aspects of NO reactivity. Complexes with transition metals:

Nitrosilation.
-Electronic structure of the Fe(II)-heme NO complexes.
-Non biological transport. Biological sources of NO: No-synthases (structure and mechanism).
-Target molecules: consequences of NO production: Ferrous hemoproteins (Guanidyl cyclase soluble (sGC), Hemoglobin (Hb), Myoglobin (Mb), Cytochrome c oxidase (CcOx), Ferric hemoproteins); Coordination centers not hemo; Dioxygen; Other radicals.
-Physiological and physiopathological levels of NO. Methods of detection of NO.

2. Coordination polymers (MOFs)

-Definition of coordination polymer (CP). Historical precedents and motivations that stimulated the initial development of the CPs. Concept of Network as a tool to describe and design CPs / MOFs. Basic units of construction of MOFs (SBUs).
-Description, classification, network topology and significant examples. Network, set of nodes and links. Topological analysis. Description and symbols for 2D, 3D and coordination polyhedra networks (Symbols of Schläfli, Vertex (M. O'Keeffe), Point (AF Wells) Examples of most common networks found in CPs: NbO, Sodalite, Diamond, Quartz (SiO2), Moganite (SiO2), SrAl2, Tri- and tetra-connected networks, etc. Means available for the topological analysis of networks in coordination polymers. Bibliography of interest on networks and CPs.
-Review of several, most significant MOFs.
-Motivations that led to the explosive expansion of the research area of MOFs.
-Selection of networks based on SBUs construction units: i) MOF-2, ii) HKUST-1, iii) MOF-14, v) MOF-5, vi) Iso-reticular series IRMOFs, vii) MOF-177, viii) Series MIL-nº: MIL-101 and MIL-5, ix) Series UiO-nº and PCN-nº, x) Series NU-nº, xi) MOFs with unsaturated coordination centers, xii) ZIFs, xiii) Covalent organic frameworks (COFs).
-Classical synthesis methods of coordination chemistry: solvothermal, mechanochemical, Sonochemical method, Solvothermal method assisted by microwaves. Activation of MOFs: lyophilization, CO2 (l) supercritical.
-MOFs photonics, catalysis, magnetic properties.

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. Organometallic chemistry

-Introduction.
-Structure and bonding.
-Compounds with sigma-donor ligands. Compounds with pi-donor ligands.
-Activation of small molecules. Compounds with P-donor ligands.
-Carbonyl metals. Metallic clusters. Wade rules.
-Iso-lobular analogy: parallelism between main-group chemistry and organometallic chemistry.
-Reactivity: i) Substitution reactions. Oxidative addition reactions. Reductive elimination reactions; ii) Insertion and elimination reactions. Addition reactions and electrophilic and nucleophilic abstraction on the coordinated ligands.
-Catalysis: Reactions with olefins and other unsaturated compounds. Industrial processes with homogeneous catalysts. Coupling reactions.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	5,00	100
Seminars	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
TOTAL	**125,00**	

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 the subject is 5.

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