COURSE DATA

Data Subject	
Code	36466
Name	Química de Coordinación
Cycle	Grade
ECTS Credits	6.0
Academic year	2019 - 2020

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	4	Second term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	16 - Inorganic Chemistry Applied	Optional

Coordination

Name	Department
LLORET PASTOR, FRANCISCO	320 - Inorganic Chemistry

SUMMARY

The aim of this optative subject is to complete the knowledge of the coordination chemistry previously acquired in the study of “Química Inorgánica III”. The study is centered in the electronic structure of the transition metal complexes, covering both theoretical (crystal field theory) and experimental aspects (absorption spectra, magnetic properties and electronic paramagnetic resonance) and also vibrational spectra (infrared and Raman).

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

It is recommended to have taken and successfully passed all the subjects in the previous courses.

OUTCOMES

1110 - Degree in Chemistry

- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them.
- Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules.
- Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications.
- Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.
- Handle chemicals safely.
- Carry out standard experimental procedures involved in synthetic and analytical work, in relation to organic and inorganic systems.
- Relate chemistry with other disciplines.
- 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.

LEARNING OUTCOMES

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Applied Inorganic Chemistry 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 Coordination Chemistry related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Coordination Chemistry that contemplate the learning outcomes EUROBACHELOR®
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 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 characteristic properties of elements and their compounds, including group relationships and trends within the Periodic Table	Interpret the variation of the characteristic properties of chemical elements according to the periodic table..(CE2). Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7).
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 properties of aliphatic, aromatic, heterocyclic and organometallic compounds.	Demonstrate knowledge of the main types of chemical reaction and their main characteristics.(CE4) Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7). Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.(CE8). Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes..(CE12).

COMPETENCES AND COGNITIVE SKILLS
The learning process should allow the degree graduates to demonstrate:

	Competences of the subject Coordination Chemistry that contemplate the learning outcomes EUROBACHELOR®
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).

On completing this course in Coordination Chemistry, students will have acquired the following skills and abilities:

Understanding and assimilation of all the concepts introduced in every topic of the program below detailed. Familiarity with the results of the calculus of the transition metals free ions electronic structure and their complexes. To be able of analyse and predict the spectral and magnetic data of a given metal.

DESCRIPTION OF CONTENTS

1. Electronic structure of atoms and ions free of the transition metals.

1.1 . - Monoelectronic approximation: electronic configurations.
1.2 .- Interelectronic repulsion: energy terms. Calculation of the terms of a configuration dx: Spin factorization method. Relative Energy of the terms: parameters of Racah.
1.3 .- Spin-orbit coupling: energy levels.
1.4 .- Effect of an external magnetic field on the energy levels of a transition metal ion: magnetic properties

2. Electronic Structure of the complexes of transition metals

2.1 .- the crystal field theory. Octahedral, tetrahedral and squared complexes.
2.2 .- Strong field approximation: electronic configurations. Comparation with the molecular orbital theory.
2.3 .- Weak field approximation: energy terms. Orgel Diagrams. Diagrams of Tanabe and Sugano.
2.4 .- Spin-orbit coupling: energy levels.

3. Electronic Spectra

3.1 .- Excited states and electronic absorption spectra. Transitions d-d. Characteristics of the absorption spectra in the visible: number, position, width and intensity of the absorption bands.
3.2 .- intensity of the absorption bands. Selection Rules: transitions from spin spin allowed and forbidden. Selection Rule of Laporte.
3.3 .- electronic transitions of spin allowed. Analysis of the absorption spectrum in the visible octohedral crystals and tetrahedral complexes of transition metals. Spin forbidden Transitions.

4. Magnetic properties

4.1.- Magnetization and Magnetic Susceptibility. Diamagnetism and paramagnetism. Van Vleck formula. Temperature-independent paramagnetism.
4.2 .- Comparative study of the magnetic moment of the complexes and free metal ions. Formula of spin only: The number of electrons molecular.
4.3 .- magnetic properties of the complex with cubic symmetry (octohedral crystals and tetrahedra). Effect of the crystal field on the magnetic moment of an ion free: partial or complete blockage of the contribution to the orbital magnetic moment. Terms A, E and T.
4.4 .- spin orbit coupling and magnetic properties. Terms A2 and E : coupling spin-orbit of second order and contribution to the orbital magnetic moment. Terms T : An Outstanding Diagrams.
4.5 .- Magnetic properties of complexes with lower symmetry (axial symmetry). Magnetic anisotropy.
4.6 .- Introduction to the spectroscopy of electronic paramagnetic resonance (EPR). Complex of Cu(II).
4.7.- Isotropic Exchange magnetic interactions: Ferromagnetism and antiferromagnetism. Magnetic susceptibility for polinuclear complexes. Orbital Models of the isotropic magnetic interaction.
4.8.- Magnetic ordering: Ferromagnetic, antiferromagnetic, ferrimagnetic and weak ferromagnetism. Slow magnetic relaxation i mono and polinuclear complexes.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Study and independent work	47,50	0
Preparation of evaluation activities	20,00	0
TOTAL	**127,50**	

TEACHING METHODOLOGY

The subject is raised so that the student is the protagonist of their own learning and is structured in the following way:

Lectures.- In these classes the teacher will give an overview of the topic object of study with special emphasis on the new aspects or particular complexity. It also will carry out the specific application of the knowledge that students have acquired via the resolution of issues and practical problems that students have previously worked. Logically, these classes will be complemented with the of personal study time of student.

Group tutoring.- Students attend them in smaller groups. In them, the teacher can propose activities, as resolution of issues or problems, resolution of doubts, approach to discussions,etc., which will contribute to the final score, as it considers the teacher.

EVALUATION

The evaluation of student learning will take into account all the aspects exposed in the methodology section of this teaching guide. The knowledge acquired during the course will be evaluated at the end of the course through an exam, on the date established by the Faculty. To pass, a minimum grade of 5 will be required.

The qualification of the second call will be adjusted to the same criterion of the first call.

REFERENCES

Basic

- S. F. A. Kettle, Physical Inorganic Chemistry. A Coordination Chemistry Approach, Spektrum Academic Publishers, Oxford, 1996.

- J. Ribas Gispert, Química de Coordinación, Edicions de la Universitat de Barcelona/Ediciones Omega, 2000 (existe una versión más reciente en inglés: Coordination Chemistry, Wiley-VCH, 2008).

Additional

- M. Gerloch, Orbitals, Terms and States, Wiley, 1986.
- B. N. Figgis and M. A. Hitchman, Ligand field theory and its applications, Wiley-VCH, 2000.
- P.S. Braterman, Spectra and Bonding in Metal Carbonyls. Part B: Spectra and Their Interpretation, en D. M. P. Mingos (ed), Structure and Bonding, Vol 26, p. 1-42, Springer, 1976.

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

1. Contenidos

Se mantienen los contenidos inicialmente recogidos en la guía docente.

2. Volumen de trabajo y planificación temporal de la docencia

Se mantiene la carga de trabajo para el estudiante que marca el número de créditos.

Se mantiene el peso de las distintas actividades que suman las horas de dedicación en créditos ECTS marcadas en la guía docente original.

Se mantienen las sesiones programadas en las mismas fechas y horas con la misma duración.

3. Metodología docente

Durante la docencia no presencial se sigue subiendo material al Aula virtual, en especial se han preparado manuscritos de los diferentes temas y se han subido al Aula virtual para que el alumno tenga todas las lecciones totalmente desarrolladas, puesto que es un poco más difícil su intervención a lo largo de las videoconferencias.

Se siguen proponiendo actividades a través del Aula virtual (ejercicios a desarrollar, ejercicios resueltos, cuestionarios, …).

La clase magistral se ha sustituido por videoconferencias (BBCollaborate) a través del Aula virtual.

Las dudas o tutorías se realizan por correo electrónico (a nivel individual) y/o por videoconferencias que se programan en función de las demandas.

4. Evaluación

Desde que se ha empezado la docencia “no presencial”, se han iniciado una serie de actividades para el alumnado (ejercicios, cuestionarios, trabajos a desarrollar) que se les entrega al principio de la semana y el alumno los entrega terminados al final de la misma para su corrección y evaluación. Esta evaluación continua tendrá un peso importante para la evaluación final: un 35 % (lo cual no estaba contemplado en la guía inicial). Se realizará una prueba escrita (tipo examen tradicional) con un tiempo límite de duración, es decir, el examen consistirá en una serie de cuestiones a desarrollar en un tiempo limitado, el profesor estará a conectado a través del aula virtual y con conexión a videoconferencia durante el desarrollo del mismo para aclarar cualquier duda (65 %). La entrega se realizará mediante escaneado o foto y se enviará por correo electrónico al profesor. Para ello, los estudiantes dispondrán de unos minutos desde que se termine el examen.

Será un requisito el aprobar este examen con una nota igual o superior a 5 sobre 10.

5. Bibliografía

La bibliografía se mantiene. Sin embargo, para evitar problemas se han escrito los temas que se van a impartir de forma no presencial y se ha entregado a los alumnos a través del Aula virtual.