COURSE DATA

Data Subject	
Code	36466
Name	Química de Coordinación
Cycle	Grade
ECTS Credits	6.0
Academic year	2018 - 2019

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.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

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 (RD 1393/2007) // NO CONTENT (RD 822/2021)

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.