VNIVERSITAT DE VALÈNCIA

Course Guide
34221 Coordination and organometallic chemistry

COURSE DATA

Data Subject	
Code	34221
Name	Coordination and organometallic chemistry
Cycle	Grade
ECTS Credits	4.5
Academic year	2016 - 2017

Study (s)

Degree	Center	Acad. year	Period
1108 - Grado de Química	Faculty of Chemistry	4	First term

Subject-matter

Degree	Subject-matter	Character
1108 - Grado de Química	16 - Applied inorganic chemistry	Optional

Coordination

Name	Department
ROMERO MARTINEZ, FRANCISCO MANUEL	320 - Inorganic Chemistry

SUMMARY

The aim of this optional subject is to supplement the knowledge of coordination and organometallic chemistry previously acquired in the compulsory subject Inorganic Chemistry III. The course focuses on the electronic structure of transition metal complexes, covering both theoretical (crystal field theory) and experimental aspects (absorption spectra, magnetic properties and electron paramagnetic resonance) and also their 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 advisable that students have successfully completed all the subjects in the previous academic years.

OUTCOMES

1108 - Grado de Química

- 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.
- Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes.
- 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

Understanding and assimilation of all the concepts introduced in every unit of the programme detailed below. Familiarity with the results of the calculations of the electronic structure of the free ions of transition metals and their complexes. Ability to analyse and predict the spectral and magnetic properties of a given metal complex.

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. Complex octohedral crystals, tetrahedra and square.
2.2.- Strong field approximation: electronic configurations. Compared to the molecular orbital theory.
2.3.- Weak field approximation: energy terms. Orgel Diagrams. Diagrams of Tanabe and Sugano.
2.4.- Coupling spin-orbit: 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: absorption spectrum of the ion [Mn(H2O)6]2 .

4. Magnetic properties

4.1.- Comparative study of the magnetic moment of the complexes and free metal ions. Formula of spin only: The number of electrons molecular.
4.2.- 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.
4.3.- 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.
4.4 .- magnetic properties of complexes with lower symmetry (axial symmetry). Magnetic anisotropy.
4.5 .- Introduction to the spectroscopy of electronic paramagnetic resonance (EPR). Complex of Cu(II).

5. Introduction to organometallic chemistry

5.1.- ligand in organometallic chemistry. Carbonyls. Similar Ligands to the CO. Hydride complexes and dihydrogen. Other small molecules.
5.2.- Link between metal atoms and organic p systems. P linear systems. P cyclical Systems.
5.3.- Complexes containing single, double and triple metal-carbon bonds: alkyl and similar complexes. Carbenes and carbynes.
5.4.- Compounds with metal-metal multiple bonds.

6. Reactivity of organometallic compounds

6.1.- Reactions involving the loss or gain of ligands. Oxidizing reactions of addition and elimination reducer.
6.2.- Reactions of modifying ligands coordinated. Insertion reactions. Reactions of adding and removing nucleofilica and electrophilic.
6.3.- Reactions of free radicals with metal complexes.

7. Applications in catalysis.

7.1.- Different types of catalysis using organometallic compounds.
7.2.- Catalytic processes more important from an industrial point of view.
7.3.- Coupling reactions.
7.4.- Asymmetric Catalysis.
7.5.- Applications in organic synthesis.

WORKLOAD

ACTIVITAT	Hours	% To be attended
Theory classes	38.00	100
Tutorials	7.00	100
Study and independent work	47.50	0
Preparation of evaluation activities	20.00	0
TOTAL	**112.50**	

TEACHING METHODOLOGY

This subject is designed so that students lead their own learning and is structured in the following components:

Lectures.- In these classes the lecturer will provide an overview of the topic under study with special emphasis on new aspects or on those particularly complex. Lessons will also involve the specific application of the knowledge acquired by students via the resolution of questions and practical problems that students must have previously worked on. Logically, these classes must be complemented with individual study.

Group tutorials.- Students attend these sessions in small groups. In them, the lecturer may propose activities such as resolution of questions or problems, answer to queries, discussions, etc. which may contribute to the final mark, at the lecturer's discretion.

EVALUATION

The knowledge acquired by students will be assessed at the end of the course through an examination on the date established by the Faculty. This will be the only evaluation procedure for all the students that choose option A. A minimum score of 5 out of 10 will be required to pass. Additionally, on a voluntary basis, one partial test will be conducted covering the first half of the programme. The students who pass it (minimum score of 5) will not be tested on this part of the programme at the end of the course. The final score will be the arithmetic mean of the marks obtained in both assessments (option B). A minimum mark of 5 out of 10 will be required to pass. Students who do not pass the partial evaluation, or those who wish to improve their mark, will be assessed as in option A. The second examination sitting will also follow option A.

REFERENCES

Basic

- Kettle,S. F. A. Physical Inorganic Chemistry. A Coordination Chemistry Approach. Spektrum Academic Publishers, Oxford, 1996. ISBN: 978-0-7167-4514-3
- Ribas Gispert,J. Química de Coordinación, Edicions de la Universitat de Barcelona/Ediciones Omega, 2000. ISBN: 9788428212106
  Existe una versión más reciente en inglés:
  Ribas Gispert,J. Coordination Chemistry, Wiley-VCH, 2008. ISBN-13 978-3-527-31802-5
- Crabtree,R.H.; Peris,E. Química Organometálica de los Metales de Transición, Castellón, Biblioteca Univ. Jaume I, 1997. ISBN: 84-8021-164-2
- Elschenbroich,C. Organometallics, 3rd. Ed., Ed. WILEY-VCH, 2005.ISBN: 3-527-29390-6

Additional

- Gerloch,M. Orbitals, Terms and States, 1ª Ed. Wiley, 1986. ISBN-13: 978-0471909354
- Figgis,B. N.; Hitchman, M. A. Ligand field theory and its applications, New York: Wiley-VCH, 2000. ISBN 0.471-31776-4
- Braterman,P.S. Spectra and Bonding in Metal Carbonyls. Part B: Spectra and Their Interpretation, en Mingos, D. M. P. (ed), Structure and Bonding, Vol 26, p. 1-42, Springer, 1976.
- Crabtree,R. H. The Organometallic Chemistry of the Transition Metals, 5th Ed., Ed. Wiley Interscience John Wiley and Sons, 2009.ISBN: 978-0-470-25762-3
- Astruc,D. Química Organometálica, !ª Ed. Barcelona: Ed. Reverté, 2003. ISBN: 84-291-7007-3