

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

Code	34200
Name	Inorganic chemistry III
Cycle	Grade
ECTS Credits	6.0
Academic year	2018 - 2019

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	3	First term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	8 - Inorganic Chemistry	Obligatory

Coordination

Name	Department
GARCIA-ESPAÑA MONSONIS, ENRIQUE	320 - Inorganic Chemistry

SUMMARY

Inorganic Chemistry III (6 credits) is a core subject included in the fundamental chemistry module and taught in the sixth term of the Degree in Chemistry.

After the study of Inorganic Chemistry I and II, where students acquire a basic knowledge of the subject matter and study the properties of chemical elements and their compounds, Inorganic Chemistry III focuses on the study of two key groups of inorganic compounds: the coordination and organometallic compounds, and solids.

The coordination and organometallic compounds play an important role in inorganic chemistry and are applicable to a wide variety of systems. Their study brings together concepts, theories, and experimental facts – and includes electronic structure and molecular synthesis and substance reactivity, thermodynamics and kinetics, basic studies, and applications. By its nature, it extends from theoretical chemistry to biochemistry and organometallic chemistry – and blurs the boundaries between the conventional inorganic and organic chemistry. The optional subject Coordination and Organometallic Chemistry (4.5 credits) in the field of applied inorganic chemistry, will complete this study.



The area of new materials is progressing very quickly and there is a marked interest in the synthesis and properties of new inorganic solids. The items included in Inorganic Chemistry III will enable the student to understand this field and is supplemented by the core subject of Materials Science (6 credits) in the seventh term.

Inorganic Chemistry III discusses symmetry and group theory, which is a useful tool in chemistry, and needed to rigorously address several aspects of the coordination compounds of transition metals.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

1108 - Degree in Chemistry V1-2009 :

1110 - Degree in Chemistry V2-2018 :

1929 - Double Degree in Physics and Chemistry :

1934 - Programa de doble Grado Química-Ingeniería Química_2023 :

R4-OBLIGATION TO HAVE SUCCESSFULLY COMPLETED THE COURSE

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

Other requirements

Students should have completed and passed the subjects I Inorganic Chemistry and Inorganic Chemistry II.

OUTCOMES

1108 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.



- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications.
- Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.
- Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Develop sustainable and environmentally friendly methods.
- 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.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES

This course will cover the following skills and outcomes related to inorganic chemistry in the degree course:

1. Relating, distinguishing, and recognising the behaviour of chemical elements and their compounds, as well as predicting the properties, link type, structure, and possible reactivity of unspecified inorganic compounds on the basis of the relationship between groups and established variations.
2. Assigning and determining the structure of various types of inorganic compounds.
3. Understanding and using bibliographic and technical information relating to inorganic compounds.
4. Explaining in an understandable way, phenomena and processes related to inorganic chemistry.
5. Demonstrating sensitivity to environmental issues.
6. Recognising and valuing chemical processes in everyday life.
7. Make decisions with rigour.
8. Solve problems with rigour.
9. Effectively performing the tasks assigned as a member of a team (with a gender perspective).
10. Demonstrating skills in interpersonal relations (with a gender perspective).
11. Demonstrating ability to use information and communication technologies.
14. Explaining in an understandable way experimental phenomena with supporting theories.
16. Demonstrating ethical commitment (with a gender perspective).
17. Demonstrating creativity.



18. Demonstrating independent learning.

At the end of the course students should be capable of:

- identifying the elements of molecular symmetry
- sorting molecules into their groups
- using character tables, primarily of the groups O_h , D_{4h} and T_d
- applying the concepts of symmetry to construct diagrams of molecular orbitals
- predicting the relative stability of two or more coordination compounds, as well as their labile or inert nature
- classifying the type of chemical reaction involving a coordination or organometallic compound
- inferring from observed behaviour the mechanism of a redox reaction in compounds of coordination
- describing the M-ligand link in organometallic compounds
- resolving coordination and organometallic chemistry problems by reasoning, idea association, and an understanding of fundamental interrelationships
- understanding the crystalline structure of different types of inorganic solids and affecting factors.
- Analysing reactions included in a catalytic cycle.
- Producing reports with the appropriate terminology, as well as making oral presentations of key aspects.
- Demonstrate an ethical and responsible conduct in the exercise of their professional work, values that are transmitted by teachers and researchers of the University, as a generator and transmitter of scientific knowledge.

DESCRIPTION OF CONTENTS

1. Molecular symmetry

- 1.1 Symmetry. Elements and symmetry operations.
- 1.2. Point groups of symmetry. C_{4v} , D_{3h} , D_{4h} T_d and O point groups.
- 1.3. Determination of the point group symmetry of a molecule.
- 1.4 Character tables. Species of symmetry. Symmetry of atomic orbitals.



2. Coordination and Organometallic transition metal compounds

2.1 General characteristics: oxidation state. Index and geometry of coordination. Square, tetrahedral and octahedral complexes. Geometry and symmetry of coordination. Idealization of the symmetry of coordination.

2.2 Types of ligands. Classification: nature of the atom giver, denticity, nature of the link metal-ligand. Ligands in Organometallic chemistry.

3. The bond nature and electronic structure

3.1 Molecular orbital theory. Molecular orbital diagrams and electron configuration of the square, tetrahedral and octahedral complexes. Link to sigma and pi bond. High-spin and low spin complexes. Excited states: types of electronic transitions.

3.2. Model of angular overlap. Diagrams of energy splitting of d-orbitals in complexes of different symmetries.

4. Molecular structure

4.1 Factors that determine the molecular structure of a metal complex: steric and electronic.

4.2. Prediction of the rate of coordination. Of the 16 and 18 electron rule.

4.3. Prediction of the geometry of coordination through the VSEPR model and the model of angular overlap. Stereochemistry of organometallic complexes.

4.4. Particular study of the various indices and geometries of coordination.

4.5 Isomerism in coordination compounds.

5. Reactions of metal complexes: thermodynamic and kinetic aspects

5.1. Reactions in coordination chemistry.

5.1.1 Substitution reactions of ligand: metal ions in aqueous solution, an exchange of water: lability and inertia. Equilibria of formation of metal complexes in solution. Stability constants. Irving series-Williams. Chelate effect. Kinetics and mechanism of substitution reactions of ligand in a complex plane and octahedral square.

5.1.2. Redox reactions: reactions of electronic transfer. Spontaneity of redox reactions: redox potential and stability constants. Mechanisms: internal and external area.

5.2. Reactions in Organometallic chemistry and catalysis. Types of reactions: substitution and dissociation reactions of ligand. Oxidative addition and reductive elimination reactions. Insertion reactions. Reactions of hydride elimination. Ciclometalación. Principles of catalysis. Catalytic processes: hydrogenation of alkenes. Hydroformylation. Monsanto acetic acid synthesis process. Waker (Smidt) process. Metathesis of olefins.

**6. INORGANIC SOLIDS: crystalline defects and not stoichiometry**

Structural imperfections in solids. Point defects. Dislocations. Burger's vector. Surface defects. Microscopic observation of defects.

Non-stoichiometry: thermodynamic and structural aspects.

7. Solid state reactivity

Diffusion in solids. Laws of diffusion. Factors affecting diffusion. Examples.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Study and independent work	70,00	0
Preparation of evaluation activities	20,00	0
TOTAL	150,00	

TEACHING METHODOLOGY

The subject is raised so that the student is the protagonist of their own learning and vertebrará around four axes:

Participatory lectures-in those classes the teacher give an overview of the topic object of study with special emphasis on the key concepts or of particular complexity. Indicate those most recommended resources that complement the topic on personal study time. The teacher will induce the student to participate in the discussions that arise through exposure of the subject.

Practical classes and seminars-these classes are carried out the specific application of the knowledge that students have acquired in theory classes. Students must previously have worked the problems will be resolved. The resolution of these problems is carried out on some occasions by the teacher and in another case by the students well in group, either on an individual basis.

Tutoring-students attend them in groups and will be one hour. In them, teacher will guide the student on the elements that make up the learning process, at the same time which will evaluate their process of learning in a global way. The student will receive a list of questions and problems that you will exercise on each of the aspects dealt with in class sessions. Also, tutorials will serve to resolve all questions that have been able to arise during classes and guide students on the methods of work more useful to the resolution of problems that may arise.



Seminars and Conference: Seminars and Conference will focus on complementary aspects of their training in Inorganic Chemistry. For this task, students attending the event and answer a questionnaire prepared by the instructor.

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

- Housecroft, C. E.; Sharpe, A. G.; Inorganic Chemistry, ed. Pearson Prentice-Hall, 3^a edició, 2008. ISBN: 978-0-13-175553-6.
(En format separat, s'ha publicat el manual de respostes als exercicis plantejats. Existeix una traducció a l'espanyol de la 2^a edició i del manual de respostes d'Ed. Pearson Prentice-Hall, 2006.)
- Atkins, P. W.; Overton, T. L.; Rourke, J. P.; Weller, M. T. y Armstrong, F. A.; Shriver & Atkins: Inorganic Chemistry, ed. Oxford, 5^a edició, 2010. ISBN: 978-0-19-923617-6.
(Existeix una traducció al espanyol de la quarta edició de Ed. McGraw-Hill, 2008).
- Rayner-Canham, G.; Overton, T.; Descriptive Inorganic Chemistry y Student solutions manual for descriptive inorganic chemistry, ed. W. H. Freeman, 4^a edició, 2006. ISBN 10: 1-4292-1814-2.
(Existeix una traducció al espanyol de la 2^a edició de G. Rayner-Canham, Química Inorgánica Descriptiva, ed. Prentice Hall, 2000)
- Miessler, G. L.; Tarr, D. A., Inorganic Chemistry, 4^a edició, ed. Pearson/Prentice Hall, 2011. ISBN-13: 978-0136128663

Additional

- Cotton, F. A.; Wilkinson, G.; Murillo, C. A.; Bochmann, M.; Advanced Inorganic Chemistry, ed. Wiley-Interscience, 6^a edició, 1999. ISBN: 978-0-471-19957-1
Existeix una traducció al espanyol de la 4^a edició, F. A. Cotton y G. Wilkinson, Química Inorgánica Avanzada, ed. Limusa, 1987.



- Greenwood, N. N.; Earnshaw, A.; Chemistry of the Elements, ed. Elsevier Science, 2ª edición, 1997 (corregida en 1998, con reimpresiones en 2001 y 2002). ISBN: 0-7506-3365-4.
- Wells, F.; "Química Inorgánica Estructural", 4ª ed. Reverté, Barcelona, 1994. ISBN-13: 978-8429175240; ISBN-10: 8429175245
- Purcell, K. F. ; Kotz, J. C.; Inorganic Chemistry, Saunders, 1977 (existe traducción al castellano, editorial Reverté).
- A.R. West, Solid State Chemistry and Its Applications, ed. John Wiley & Sons, 1987 (edición corregida de la publicada en 1984). ISBN: 0 -471-9037709
- Greenwood, N. N.; Cristales iónicos, defectos reticulares y no estequiometría, 1ª ed. Madrid: ed. Alhambra, 1970. ISBN: N.A.