

Bachelor's Degree in Chemistry

Subject Guide

1. Information about the subject

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|------------------------------|--|-------------------------|---------------------|
| SUBJECT | Concepts and Models in Inorganic Chemistry | CODE | GQUIMI01-2-005 |
| EDUCATIONAL OFFER | Bachelor's Degree in Chemistry | CENTER | Facultad de Química |
| TYPE | Compulsory | N° TOTAL CREDITS | 6.0 |
| PERIOD | First Semester | LANGUAGE | Spanish |
| COORDINATORS/ES | | EMAIL | |
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2. Context

The course is given in the first semester of the second year of the Degree in Chemistry, and is part of the Degree Basic Module (Inorganic Chemistry part). It is a theoretical course. The course objective is to provide all the necessary concepts needed to describe the structure and bonding of the chemical elements and inorganic compounds in order to understand the existent relationship between structure/bonding and properties/reactivity. The student will also learn the basics of inorganic and coordination chemistry nomenclature.

The concepts acquired in this course are essential to other courses, such as "Chemistry of the Representative Elements" (CRE, 2^o year, 2^o semester) and "Chemistry of the Transition Elements" (CTE, 3^o year, 2^o semester), and very useful for the experimental course "Experimentation in Inorganic Chemistry I" (3^o year, 1^o semester).

The course will be taught by professors from the area of inorganic chemistry (Department of Organic and Inorganic Chemistry of the University of Oviedo).

3. Requirements

Since this course is part of the Degree Basic Module, to register for this course it is necessary to have passed the first year courses "General Chemistry" and "Laboratory Operations and Computing Tools".

4. Competencies and learning results

The generic and specific course competences according to the Inorganic Chemistry part of the Degree Basic Module (see verification report) are:

Generic competences:

- Develop the ability for analysis and synthesis (CG-1).
- Solve problems effectively (CG-2).
- Adequate information management (CG-6).
- Proper communication (speaking and writing) in English (CG-8).
- Independent learning (CG-9).
- Develop critical reasoning (CG-17).
- Teamwork (CG-18).

Specific competences-Knowledge:

- To consolidate the knowledge about fundamentals of chemical terminology, nomenclature and units (CE-1).

- To correlate the macroscopic properties with those of the atoms and molecules constituents of matter (CE-2).
- Recognise the variation of the periodic properties of the chemical elements (CE-3).
- Describe the types of chemical reactions and their associated characteristics (CE-5).

Specific competences-Skills:

- Capability to understand and explain those essential facts, concepts and principles related to the field of chemistry (CE-19).
- Solve quantitative and qualitative problems according to previously developed models (CE-20).
- Acquire skills to evaluate, interpret and summarise chemical information (CE-22).
- To use correctly inductive and deductive methods in the field of chemistry (CE-32).

The **expected learning outcomes** will be:

- Know how to use the criteria and methods needed to describe the structures of inorganic compounds.
- Be able to describe the most representative structures of inorganic compounds with or without external aids such as models or appropriate software.
- Learn the concept of molecular symmetry and know the symbols used to describe it, know how to classify molecules according to their specific symmetry and how to use and interpret the character tables.
- Be capable of drawing Lewis Structures, including representative canonical forms, of inorganic molecules and using VSEPR model to determine their three-dimensional shape.
- Know and use the molecular orbital (MO) diagrams of common molecules to predict their properties according to a specific electronic configuration.

- Be able to describe the bonding nature of metallic, covalent and ionic solids in order to explain their different properties, especially regarding conductivity.
- Considering the different valency and electronegativity of the elements, be able to identify the composition (formula), structure and bonding in inorganic compounds.
- Be able to write down the correct chemical formula and name (trivial, semi-systematic and/or systematic) of inorganic compounds.
- Relate the properties of the substances, particularly melting and boiling points and solubility, with their chemical composition.
- Know the main types of inorganic chemistry reactions, for discrete molecules and also for solids, and explain the possible results according to kinetic and thermodynamic aspects.
- Learn the basics of coordination chemistry knowing nomenclature, structure and bonding in coordination compounds. Classify known and potential ligands. Know how to determine the magnetic properties of complexes. Know how to evaluate the lability or inertia of complexes and the kinetics in redox reactions.

5. Contents

The course is divided into 7 lessons, whose contents are summarised as follows:

LESSON 1. Structure of elements and compounds. Structure of solids. Interatomic distance interpretation. Types of solids. Structures of molecules and of ionic units. Structures of non-molecular solids. Unit cell. Close-packed structures. Polyhedron packing. Representative structures and anti-structures. Structures of CaF₂, NaCl, ZnS blende, CaF₂, NiAs, CdI₂, ZnS wurtzite, rutile, β-cristobalite, corundum, ilmenite, perovskite and spinel. Real structures. Point-defects. Non-stoichiometric compounds.

LESSON 2. Symmetry. Symmetry operations and elements. Symmetry elements in molecules. Structure and symmetry. Classification of molecules according to their symmetry. Character tables. Orbitals symmetry.

LESSON 3. Bonding in elements and compounds. Bonding description in molecules using valence bond (VB) theory. Lewis structures. VSEPR model. Resonance in VB bonding: major canonical forms. Bonding descriptions in molecules using molecular orbital (MO) theory. Qualitative and semi-empirical MO diagrams. Electronic configuration in molecules. Diatomic molecules. F₂, O₂, N₂, HCl, CO and related molecules. Polyatomic molecules: H₂O, NH₃, SO₂, CO₂, SO₃ and related molecules. Electron deficient multi-centred bonds: B₂H₆. Electronegativity. Mulliken-Jaffé scale. Bonding in non-molecular solids. Band theory. Metallic bonding. Bonding in covalent solids. Conductors, semiconductors and insulators. Bonding in ionic solids. Lattice energy. Partial covalent character. Fajan's rule.

Valence and oxidation state. Structure and bonding of chemical elements.

LESSON 4. Introduction to inorganic chemistry nomenclature and formulae. Binary compounds. Compounds containing hydrogen. Compounds containing polyatomic anions and/or cations. Ternary compounds. Oxoacids. Oxosalts.

LESSON 5. Relationship between structure and properties. Melting and boiling points in molecular and non-molecular substances. Intermolecular cohesive effects: hydrogen bonding. Solubility and miscibility. Solubility of salts in water. Qualitative rules.

LESSON 6. Introduction to inorganic chemistry reactions. Generic types of reactions. Thermodynamic versus kinetic reaction control. Reactions between discrete species in the gaseous phase and in solution. Addition reactions. Simple addition. Lewis acids and bases. Hard and soft acids. Addition followed by elimination reactions: solvolysis. Insertion reactions. Oxidative addition reactions. Substitution reactions. Metathesis reactions (or exchange reactions). Metathesis reactions between salts: precipitation. Reorganization reactions: isomerisations. Proton transfer reactions. Reduction-oxidation reactions. Analysis using oxidation state diagrams. Reactions of elements with acids. Reactions between non-molecular solids. Kinetic and thermodynamic factors. Analysis using phase diagrams.

LESSON 7. Coordination chemistry. Coordination compounds. Nomenclature and formulae. Ligands classification. Coordination number and structure. Isomerism. Stereoisomerism. Bonding in coordination compounds. Electronic configuration and properties using crystal field theory (CFT). Spectrochemical series. Magnetic properties of complexes. Jahn-Teller distortion. Electronic configuration and structure. Preference energies. Spinel and inverted spinel. Complexes stability. Stability constants. Chelate and macrocyclic effects. Reactions of coordination complexes. Substitution reactions: mechanisms. Labile and inert complexes. Substitution in square-planar complexes: trans-effect. Electron transfer reactions. Inner and outer sphere mechanisms. Reaction rate rationalization.

6. Methodology and working plan

The methodology used to achieve the competences and learning outcomes proposed will be based on:

1. **Lecture classes (LC):** In these classes the teacher will present and discuss the subject matter of study providing all the material needed (datasheets, power point-slides, etc.)
2. **Problem classes (PC):** These classes will be focused on solving specific problems/questions related to the course contents and to answer questions raised by the students.
3. **Tutorial classes (TC):** A series of questions and problems will be proposed in advance, which will be solved and discussed by the students during these classes. Additionally, short written tests with questions related to those proposed in advanced will be carried out in these classes to evaluate that lecture material is being absorbed. Students are expected to be able to adequately solve the tasks proposed and to answer the questions made in written tests.

In all classes, power-point presentations and slides using an overhead projector will be used, and/or writing on the classroom board. All the questions/problems

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|---|------------|----|---|--|--|---|---|---|-----------|--|-----------|----------|
| LESSON 3. Bonding | | 11 | 1 | | | 1 | | | | | 22 | |
| LESSON 4. Nomenclature | | 3 | | | | | | | | | 5 | |
| LESSON 5. Structure/properties | | 2 | 1 | | | | | | | | 5 | |
| LESSON 6. Reactions | | 6 | 1 | | | 1 | | | | | 14 | |
| LESSON 7. Coordination chemistry | | 10 | 2 | | | 1 | | | | | 22 | |
| | | | | | | | | | | | | |
| Total hours | 150 | 42 | 7 | | | 4 | 4 | 3 | 60 | | 90 | 9 |

| CATEGORIES | | Hours | % | Total |
|----------------------------|---|--------------|----------|--------------|
| ATTENDANCE WORK | Lecture classes | 42 | 28 | |
| | <i>Problem classes / seminars / workshops</i> | 7 | 4.67 | |

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|--|--|-----|------|--|
| | <i>Laboratory work / computing classes / field work / language classes</i> | | | |
| | <i>Medical training classes</i> | | | |
| | <i>Tutorial classes</i> | 4 | 2,67 | |
| | <i>External work</i> | 4 | 2,67 | |
| | <i>Evaluation and assessment</i> | 3 | 2.00 | |
| AUTONOMOUS STUDENT LEARNING | <i>Teamwork</i> | | | |
| | <i>Individual work</i> | 90 | 60 | |
| | Total hours | 150 | | |

7. Evaluation of the student's learning results

Grading and assessing of students learning will be carried out by means of a written exam at the end of the semester (80 % of total mark) and by participation of students in the TC classes (20 % of total mark). The total mark [(exam mark out of 10 points x 0.8) + (TC classes mark out of 10 points x 0.2)] must be equal or higher than 5 points to pass the course.

In the extraordinary calls the evaluation will be based exclusively on the result of a written exam. Again, a mark equal or higher than 5 points (out of 10) is required to pass the course.

8. Resources, bibliography and complementary documentation

The contents of the course are based on several books, however, the following textbook is recommended as the best available:

- **Gabino A. Carriedo** *“Introducción a la Química Inorgánica”*. 5ª Edición. Servicio de Publicaciones de la Universidad de Oviedo. **2011**.

Other alternative textbooks are:

- **A. F. Holleman, E. Wiberg** *“Inorganic chemistry”*. Academic Press. N.Y. **2001**.

- **J. E. Huheey, E. A. Keiter and R. L. Keiter** *“Inorganic Chemistry: Principles of Structure and Reactivity”*. 4th edition. Pearson, **1993**.

- **P. F. Schriver, P. W. Atkins, T. L. Overton, J. Rourke, M. Weller, F. Armstrong** *“Inorganic Chemistry”*. 5th edition. Oxford University Press, **2010**.

