Universitat Autònoma de Barcelona

2023/2024

Chemistry Fundamentals

Code: 102447
ECTS Credits: 6

Degree	Type	Year	Semester
2500897 Chemical Engineering	FB	1	1

Contact

Name: Ricard Gelabert Peiri

Email: ricard.gelabert@uab.cat

Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

Ricard Gelabert Peiri

Prerequisites

It is highly advisable that prior to taking this subject the student has learnt to formulate and name inorganic compounds, and understands basic concepts in chemistry, such as: mole, valence, oxidation state, and balancing chemical equations, and is able to perform stoichiometric calculations.

Objectives and Contextualisation

This subject aims at providing the student with a conceptual basis of the foundations of chemistry. The subject is made up of four different parts. In the first part a brief *review* of concepts that should have been mastered during high school, such as formulation and naming of inorganic compounds, common types of chemical reactions, chemical reaction balancing and how to perform stoichiometric calculations. The second part changes perspective and takes on an atomistic approach, and studies the quantum mechanical description of the hydrogen atom, and uses it to explain the electronic structure of many-electron atoms and in the end, the periodic table. The third part deals with the characteristics of the different chemical bond types, goes on to molecular structure and how this can be used to explain the appearance of intermolecular forces and the effect of these. Finally, the fourth part deals with solids, explains the structure of crystalline solids with special emphasis on ionic solids (but by no means only ionic solids!)

The following are the general goals of this subject. After passing the subject the student ought to be able:

- to carry out stoichiometric calculations associated to relatively complex reactions and processes, as well as to name and formulate simple inorganic compounds.

- to correctly interpret the concept of hydrogenoid atomic orbital, to be able to draw representations of them and recognize their form, and to perform simple quantitative calculations with them, determining directions and distances of maximum probability.

- to predict the electron configuration of atoms and ions, and to discuss the periodic properties of chemical elements depending on it.

- to distinguish the different bond types and to describe them using the different theories available.

- to predict the grometry of covalent molecules as well as to determine the existence (and if so, intensity) of possible polarities.

- to predict the kind and intensity of intermolecular forces between discrete molecules, and the consequences of these in terms of macroscopic properties of the substances.

- to identify the most usual crystalline structures and to compute their properties, such as coordination numbers of constituting atoms, density or, for ionic crystals, their lattice energy.

Competences

- Apply relevant knowledge of the basic sciences, such as mathematics, chemistry, physics and biology, and the principles of economics, biochemistry, statistics and material science, to comprehend, describe and resolve typical chemical engineering problems.
- Apply scientific method to systems in which chemical, physical or biological transformations are produced both on a microscopic and macroscopic scale.
- Develop thinking habits.
- Students must be capable of applying their knowledge to their work or vocation in a professional way and they should have building arguments and problem resolution skills within their area of study.
- Students must have and understand knowledge of an area of study built on the basis of general secondary education, and while it relies on some advanced textbooks it also includes some aspects coming from the forefront of its field of study.

Learning Outcomes

1. Apply scientific method to the fields of dissolution equilibrium and organic chemistry.
2. Apply standards when naming chemical compounds and recognise the different ways of expressing concentrations in dissolution.
3. Apply the different bonding theories to molecules to deduce their structure, geometry and physical and chemical properties and understand the advantages and limitations of each.
4. Describe the basic principles of quantum mechanics, the physical meaning of quantum numbers and their effect on the quantification of energy.
5. Develop a capacity for analysis, synthesis and prospection.
6. Develop critical thinking and reasoning
7. Explain the origin of the order of the chemical elements in the periodic table and how different periodic properties vary via the periodic table.
8. Identify the different types of chemical reaction and properly equate the corresponding equations.
9. Interpret the nature of the different types of bonding in metallic solids and apply the consequences to the interpretation of their structure and properties.
10. Interpret the physical meaning of the orbital wave function and apply the principles of energy quantification to the generation of the different orbital functions of hydrogenoid and non-hydrogenoid atoms.
11. Students must have and understand knowledge of an area of study built on the basis of general secondary education, and while it relies on some advanced textbooks it also includes some aspects coming from the forefront of its field of study.

12. Summarise the behaviour of gases and the different laws that describe them.

Content

Part I: Basic Concepts

- Unit 1: Matter and Chemical Compounds. Matter and substance. Properties of matter. Measurement of properties. Basic laws of chemistry. Mole. Isotopes. Molecular mass. Compossition. Empirical and molecular formulae. Solutions. Oxidation states. Naming and formulation of inorganic compounds.

- Unit 2: Introduction to Chemical Reactions. Chemical reactions. Equation balancing. Stoichiometric calculations. Limiting reagent. Electrolytes. Precipitation and acid-base reactions. Strong and weak acids and bases. Conjugate acids and bases. Redox reactions. Balancing of redox reactions in acid and basic media.

Part II: Atomic Structure

- Unit 3: The Hydrogen Atom. Concepts of classical physics. Waves and particles. Electromagnetic radiation. Historic background to quantum mechanics. Planck's, Einstein's and de Broglie's hypotheses. Wave-particle duality. Atomic models. Quantum mechanical description of the hydrogen atom. Hydrogenoid orbitals. Quantum numbers. Energy quantization. Energy degeneracy. Representations of the hydrogenoid orbitals. Radial distribution function. Electron spin.

- Unit 4: Many-Electron Atoms. The many-electron problem. Orbital approximation. Pauli exclusion principle. Electron shielding and effective nuclear charge. Orbital penetration. Electron configuration: Aufbau principle. Hund's rule. Periodic variation of element properties: atomic and ionic radii, ionization energy, electron affinity. Electronegativity. Magnetic properties.

Part III: Molecular Structure

- Unit 5: Chemical Bond. Covalent, ionic and metallic bonding. Approximate treatment of the covalent bond: Lewis'theory. Lewis structures. Ressonance. Molecular geometry: Valence Shell Electron Pair Repulsion (VSEPR) theory. Dipole moment. Bond distance. Bond energy. Quantum mechanical description of chemical bonding: Molecular orbital theory. The Linear Combination of Atomic Orbitals (MO-LCAO) approximation. Diatomics. Ionic bond. Metallic bond. Annex: some concepts of valence-bond theory.

- Unit 6: Intermolecular Forces. Intra- and intermolecular forces. Origin of intermolecular forces. Ion-ion, ion-permanent dipole, permanent dipole-permanent dipole, and permanent dipole-induced dipoleforces. Dispersion forces. Hydrogen bonds. Effects of intermolecular interactions: phase change temperatures, solubility.

Part IV: Solid State.

- Unit 7: Solid State. Amorphous and crystalline solids. Crystalline systems. Unit cell. Cell parameters. Metallic solids. Packing systems: close packing and non-close packing. Ionic solids. Ionic crystal structures. Radius ratio rule. Lattice energy. Covalent solids. Molecular solids.

Methodology

This subject makes use of three kinds of activities: theory lectures, problem solving sessions and seminars.

Theory lectures (2 h per week) will be used to develop the theoretical content of the subject using visual materials where appropriate. This material, if used, will be made available to students through the Campus Virtual platform. Besides, audiovisual material is available for asynchronous streaming, and could be used at the lecturer's discretion as complementary material or instead of presential lecturing, especially on the review lectures.

Problem solving sessions (1 h per week) are carried out in reduced groups. At the beginning of the term a collection of exercises covering the entire syllabus will be made available through the Campus Virtual platform, along with a solution set. As theory lectures progress, some of these exercises will be solved in detail in these sessions.

A number of seminars will be scheduled thoughout the semester. In these seminars a variety of activities could be carried out, at the lecturer's discretion and based on the requests of students (if any): solving students' queries, discuss some exercise, or read and discuss some selected texts related to the syllabus. In some seminars evaluation exercises will be proposed to be done on the spot and will be part of the grade of the course.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Problem Solving Sessions	15	0.6	1, 3, 2, 4, 5, 6, 7, 8, 9, 12
Seminars	6	0.24	1, 5, 6
Theory Lectures	30	1.2	1, 3, 2, 4, 5, 6, 7, 8, 9, 12
Type: Supervised			
Problem Solving	24	0.96	1, 3, 2, 4, 5, 6, 7, 8, 9, 12
Type: Autonomous			
Personal Study	45	1.8	3, 2, 4, 7, 8, 9, 12

Assessment

Continuous Evaluation

The final grade of the subject will be computed with contributions ofthree evaluatable items: written tests, evidences and seminars

- Written Tests: These have a total weight of 60% in the final grade of the subject. A total of three tests will be scheduled, two of them partial (one of which at about mid-term, the other at the end, and both with equal weighting in the final grade: 30%) and a supplemental exam. The two partial exams will cover approximately half of the syllabus each, while the supplemental exam will cover it in full. To be able to use the scores of all items detailed in this document, a student must score at least 4.0 out of 10.0 marks in each of the partial exams. Should the student not achieve this score in any of the partial tests, s/he must take the supplemental exam to be in a position to pass the subject, where again a minimum score of 4.0 out of 10.0 must be obtained to be allowed to use the scores of the rest of items.

- Evidences: These have a total weight of 25% in the final grade of the subject. As the course progresses some more ellaborate exercises will be proposed. These are individual exercises and are usually to take home and in that case they must be turned in within a deadline. The weight of each exercise in this set is not necessarily the same and may vary according to the difficulty of the individual exercises proposed.

- Seminars: They have a weight of 15% towards the final grade. At convenient times of the syllabus assessment activities will take place in specific seminars (or all of them). These will be publicized in advance.

Single Evaluation

Students who have chosen to take the Single Evaluation itinerary will have to write two written exams on the same day therest of students take the second partial exam:

- The first exam will cover the complete syllabus of the subject (theory and exercises). The grade obtained in this exam will be their grade on Theory Contents.

- The second exam will be a short test on the contents that have been treated in the seminars. The grade of this test will be the student's grade on Seminar Contents.

To have a possibility to pass the subject the student must achieve a minimum grade of 4.0 out of 10.0 in the Theory Contents exam, and a minimum grade of 5.0 out of 10.0 in the final grade using this formula:

Final Grade = (85×Theory Contents + 15×Seminar contents)/100

If the grade of the Theory Contents is less than 4.0 out of 10.0 or the Final Grade is less than 5.0 out of 10.0 the student has a second chance to pass the subject by taking the supplemental exam to be held on a date proposed by the Degree Coordinator. This supplemental exam permits to recover only the 85% part of the Final Grade that represents the Theory Contents. The grade of the Seminar Contents cannot be recovered. The Final Grade is computed using the formula above if and only if the Theory Contents grade is at least of 4.0 out of 10.0: if the grade of Theory Contents is less than 4.0 out of 10.0 the student cannot pass the subject irrespective on the grade in the Seminar Contents.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	25%	15	0.6	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 12
Seminars	15%	9	0.36	1, 3, 2, 4, 7, 8, 9, 11, 12
Written Tests	60%	6	0.24	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 11, 12

Bibliography

These two books are equally suited:

- R. H. Petrucci, F. G. Herring, J. D. Madura, C. Bissonnette, *Química General: Principios y Aplicaciones Modernas*, Pearson, 11ª Ed, 2017, ISBN: 978-8490355336. Electronic version available at UAB.. English text: R. H. Petrucci, F. G. Herring, J. D. Madura, C. Bissonnette, *General Chemistry: Principles and Modern Applications*, Pearson, 11th Ed, 2017, ISBN: 978-0132931281.

- R. Chang, *Fundamentos de Química,* McGraw-Hill, 2011. ISBN: 978-6071505415.

Software

The use of specialized software is not foreseen. However, to visualize molecular structures or unit cells of solids when the use of physical models in the lecture room is not convenient/possible or for students with difficulties with space perception, some computer programs to represent molecular structures in space can be used (for instance, JMol). In such cases (or others that might arise) instructions to download, install and use these programs will be published via the Campus Virtual platform, and the software used will be freely distributable (shareware or freeware).