Universitat Autònoma de Barcelona

2019/2020

Chemistry Fundamentals

Code: 102447
ECTS Credits: 6

Degree	Type	Year	Semester
2500897 Chemical Engineering	FB	1	1

Contact

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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

Teachers

Ricard Gelabert Peiri

Prerequisites

It is convenient that the student has knowledge on inorganic chemistry formulation as well as on basic topics on chemical reactions (mol concept, reaction balancing, stoichiometric calculations...)

Objectives and Contextualisation

The subject is divided into four different parts. In the first part some concepts that should have been learned in High School are glossed over, such as basic formulation and chemical nomenclatre, chemical equation balancing, and stoichiometric calculations. In the second part the electronic structure theory is studied and permits to settle the foundations to study chemical bonding in molecules (third part) and solids (fourth part).

In this way, the subject has four basic goals:

1. To be able to carry out stoichiometric computations on chemical reacions and relatively complex processes.
2. To discuss the periodic properties of the chemical elements and to relate them to their electronic structure.
3. To distinguish the different kinds of bonding and to describe them using the different theories available.
4. To know the most usual crystal structures and to analyze their most important properites, such as the coordination number of the different atoms, their density or reticular 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.

- Apply the acquired knowledge and skills to develop a chemical engineering project.
- Develop thinking habits.

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. Summarise the behaviour of gases and the different laws that describe them.
12. Use the knowledge acquired in the design of analyses and processes.

Content

Part I: Inorganic nomenclature. Stoichiometry.

Unit 1: Matter and Chemical compounds. Composition of matter. Nomenclature and formulation of inorganic compounds. Measurement of the properties of matter. Dissolutions: measurements of concentration.

Unit 2: Introduction to chemical reactions. Chemical reactions and stoichiometric calculations. Chemical reactions in solution: precipitation, acid-base and redox.

Part II: Atomic Structure.

Unit 3: Hydrogenoid atoms. Electromagnetic radiation. Wave-particle duality. Uncertainty principle. Wave function and energy levels. Hydrogenoid atoms. Quantum numbers and orbitals.

Unit 4: Poliatomic atoms. Electronic configurations and periodic table. Classification of the elements. Periodicity and periodic table. Atomic and ionic radii. Ionization energy. Electron affinity. Electronegativity.

Part III: Chemical bonding in molecular systems.

Unit 5: Lewis Theory. Covalent bond, ionic bond and metalic bond. Lewis structures. Molecular geometry. Theory of valence shell electron pair repulsion. Dipole moment Bond distance. Bond energy.

Unit 6: Valence bond theory. Pi, sigma and delta bonds. Orbital overlap. Hybrid orbitals. Most common hybrid orbitals.

Unit 7: Molecular orbital theory. Molecular orbital. Approximation of the linear combination of atomic orbitals. Diatomics. H2A molecules.

Parte IV: Structure of Crystalline solids.

Unit 8: Introuction to solids and molecular solids. Types of solids: molecular, covalent, ionic and metallic. Intermolecular forces in liquids and solids.

Unit 9: Bonding in metals. Structure of metallic solids. Simple cubic packing, face centered cubic packing and compact packings. Band theory: metals, semiconductos and insulators.

Unit 10: Bonding in ionic solids. Ionic crystalline structures. Coordination number. Radius rule. Reticular energy.

Methodology

MAsterclasses (2 hours a week); problem solving classes (1 h a week); seminars to go voer past material and put the materials covered in context.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Exercise lectures	15	0.6	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 11, 12
Seminars	6	0.24	1, 5, 6, 12
Theory lectures	30	1.2	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 11, 12
Type: Supervised			
Problem solving	23	0.92	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 11, 12
Type: Autonomous			
Personal Study	45	1.8	3, 2, 4, 7, 8, 10, 9, 11

Assessment

Written tests:

These have a weight of 60% in the final grade of the subject. Three exams will be scheduled along the course, two of them will be partial exams (one towards mid term, the other to the end, both with equal weighting) and one final exam. The two partial exams will cover approximately half of the syllabus each. To be able to get your grade averaging all items in this description, it is necessary that the student obtains at least 4.5 points out of 10 in each of the partial exams. If this is not achieven in at least one of the partial exams, then the student MUST take the final exam, where again at least a grade of 4.5 out of 10.0 is required in order to be allowed to get your grade as the weighted average of the different items detailed inthis guide.

Evidences:

They count towards 20% of the final grade of the subject. Along the course some exercises will be programmed (in a number not fixed beforehand) to be solved at home and be delivered on an individual basis after some days to be corrected. The weight of each exercise can vary to represent the different difficulty posed by each of them.

Self Test Activities:

These represent 10% of the grade of the subject. In selected moments during the course some self-test activities will be proposed, usually via the Moodle platform, where they will be available for a period of time known in advance.

Group Activity:

This activity represents 10% of the grade. Students will be distributed in groups whose size will depend on the number of enrolled students (4 to 6), and will be assigned a single subject explained in the syllabus to carry out an activity in a as-yet undetermined format (written document, oral presentation, video, etc.) This activity will be programmed towards the end of the term to guarantee that most of the syllabus be already taught by then. The grade of this activity will reflect not only the academic correction of the contents and the formal aspects of the presentation, but also the equitative contribution of all students involved.

Note: Students enrolled for second or later times:

Students enrolled in this subject for a second or later time and that have failed to pass it despite having taken part in the evaluation (that is, who have a numeric grade from past years, below 5.0) have the option to show up only at the written tests (partial, or final if need be). In this case, the final grade of these students will be 100% that coming from the partial exams (or final exam) computed as set forth in the "Written tests" section above, disregarding any other activity they could have done this academic year or on past ones. Please note that in this case, to pass the subject a minimum grade of 5.0 over 10.0 is necessary, as no other items contribute to the grade. Students choosing this evaluation venue must inform the lecturer in charge in written form (E-Mail) before the first partial exam is held.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	20%	15	0.6	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 11, 12
Group Activity	10%	5	0.2	1, 3, 2, 5, 6, 8, 9, 12
Self Test Activities	10%	5	0.2	1, 3, 2, 4, 7, 8, 10, 9, 11, 12
Written Tests	60%	6	0.24	1, 3, 2, 4, 5, 6, 7, 8, 10, 9, 11, 12

Bibliography

Basic Bibliography

- R. H. Petrucci, W. S. Harwood, F. G. Herring, *Química General*, Ed. Pearson, 10ª Ed. (2011). ISBN: 978-8483226803 (disponible en versió electrònica a la xarxa de la UAB). Hi ha una edició més recent (11ª Ed., 2017), ISBN: 978-8490355336.
- R. Chang, *Fundamentos de Química,* Ed. McGraw-Hill (2011). ISBN: 978-6071505415.
- P. Atkins, *Principios de Química*, Ed. Panamericana, 5ª Ed. (2010). ISBN: 978-9500602822.