

Academic Year: ( 2017 / 2018 )

Review date: 16-05-2016

Department assigned to the subject: Materials Science and Engineering and Chemical Engineering Department

Coordinating teacher: BASELGA LLIDO, JUAN

Type: Basic Core ECTS Credits : 6.0

Year : 1 Semester : 1

Branch of knowledge: Engineering and Architecture

**REQUIREMENTS (SUBJECTS THAT ARE ASSUMED TO BE KNOWN)**

High school chemistry

**OBJECTIVES**

To understand the fundamental principles of chemistry: structure of matter, chemical thermodynamics, kinetics and chemical equilibrium

To know the reactivity of the principal organic chemical groups

To know the structure and properties of the principal macromolecules of biological interest.

To be able to handle simple analytical instruments as well as to interpret experimental results

During the course students will work on the following capabilities:

- Capability to solve complex problems
- Capability to find, understand and discriminate the relevant information to make a proper decision
- Capability to apply multidisciplinary knowledge to solve a given problem
- Capability for team work: to accept tasks and to distribute tasks among classmates to face complex problems

A collaborative attitude will be developed along the course to obtain from other agents skills and knowledge necessary for specific objectives.

**DESCRIPTION OF CONTENTS: PROGRAMME**

0. Preliminary concepts. What is chemistry? Definitions. Units. Standard conditions. Atoms. Molecules. Mole. Molecular mass. Chemical equations. Reactions in aqueous media: acids and bases, redox reactions
1. Atoms. Ancient ideas about atoms. Bohr's model. Experiments and concepts that led to Bohr's model. Foundations of quantum theory. Hydrogen atom: quantum numbers, electronic configuration, atomic orbitals, energy of hydrogen atom. Multielectronic atoms. Periodic table and periodic properties
2. Molecules. Preliminaries on covalent bonding theory: Lewis structures, molecular geometry, bond parameters, ionic character of bonds. Introduction to the theory of molecular orbitals. Visualization of molecular orbitals from valence bond theory. Simple energy diagrams. Hybridization. Coordination compounds. Intermolecular forces: coulombic and polarization forces. Hydrogen bonding. The structure of water.
3. States of matter. Aggregation states: long and short range order. Solids: ionic, metals, covalent, molecular. Gases: kinetic theory of gases, equation of state. Real gases: liquefaction. Liquids: viscosity, surface tension. Liquid crystals: membranes. Liquid vapor equilibrium: Clausius equation, equilibrium phase diagrams. Solutions: solubility, colligative properties of electrolytes and non-electrolytes.
4. Thermochemistry. Definitions: system, state variable, state function, heat and work, reversible process. First law of thermodynamics: enthalpy, heat capacity, reaction enthalpy, temperature dependence of reaction enthalpy. Second law of thermodynamics: entropy, reaction entropy, temperature dependence of reaction entropy. Third law of thermodynamics. Gibbs free energy: spontaneity, standard free energy of formation, relation between free energy and chemical equilibrium for ideal gas mixtures.
5. Equilibrium reactions. Gases: equilibrium constant, heterogeneous equilibria, factors affecting chemical equilibrium (pressure, temperature, concentration, inert gases, temperature). Arrhenius, Brønsted-Lowry and Lewis theories of acids and bases. Water self-ionization. Strength of acids and bases. Conjugate acids and bases. Hydrolysis. Buffers. Titration. Solubility. Electrochemical reactions: reducing and oxidizing agents. Balance of redox reactions. Electrochemical cells: conventions, galvanic potential, standard electrode potential, free energy and electrode potential. Electrolytic cells: Faraday's

laws.

6. Chemical kinetics. Reaction rate law. Differential and integrated reaction rates. Reaction mechanism: elemental process, molecularity, limiting reactant, reaction intermediate. Rate constants and equilibrium constants. Collision theory. Transition state theory. Catalysis: homogeneous and heterogeneous. Enzymatic catalysis: Michaelis-Menten kinetics.

7. Introduction to organic chemistry. Naming organic compounds. Empirical, molecular and structural formula. Conformational isomerism. Stereoisomerism: optical activity. Fisher projections. Molecular structure and intermolecular forces. Electronic shifts on  $\sigma$  and  $\pi$  bonds. Aromaticity. Substitution effects in  $\pi$  systems. Intermediates: radicals, carbocations, carbanions. Intermediate stability: induction, resonance, hyperconjugation. Organic reactions: classification and definitions. Substitution. Addition. Elimination. Transposition. Condensation.

8. Alkanes: reactivity. Cycloalkanes: synthesis. Alkenes: isomerism, terpenes, addition reactions (Markovnikov), oxidation and autoxidation reactions. Alkynes: electrophilic addition reactions. Aromatic hydrocarbons: addition reactions and stability, electrophilic substitution. Benzene derivatives. Alcohols and phenols: acidity, electrophilic substitution, oxidation, stability of phenoxy radicals. Ethers: reactivity and synthesis. Thiols: reactivity and synthesis. Carbonyl compounds: resonance, oxidation and reduction, nucleophilic addition, synthesis. Carboxylic acids: stability of carboxylate anion, acidity, nucleophilic substitution, synthesis. Derivatives of carboxylic compounds, acyl chlorides, esters, anhydrides, amides: nucleophilic substitution. Amines: basicity, synthesis, reactivity.

## LEARNING ACTIVITIES AND METHODOLOGY

Lectures, collective tutorials, individual tutorials and homework; oriented to attainment of theoretical knowledge. Problem solving lectures in small groups, laboratory practicals, individual tutorials and home work; oriented to attainment of practical knowledge and skills related with the syllabus

## ASSESSMENT SYSTEM

Continuous assesment:

80% Quizzes

20% Laboratory practicals

Mid term exam.

Final exam: 60% global mark. It is necessary to obtain 4 as a minimum grade in the final exam to average with continuous assesment

<b>% end-of-term-examination:</b>	60
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<b>% of continuous assessment (assignments, laboratory, practicals...):</b>	40
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## BASIC BIBLIOGRAPHY

- B.M MAHAN, R.J. MYERS Química. Curso Universitario, Addison-Wesley Iberoamericana.
- Bettelheim, Brown, Campbell, Farrell Introduction to General, Organic and Biochemistry, Brooks/Cole, 2010
- J. FISHER, J.R.P. ARNOLD Chemistry for Biologists, Taylor & Francis, 2004
- P. ATKINS, L. JONES Principios de química, Editorial Médica Panamericana.