Universitat Autònoma de Barcelona

2022/2023

Organic Chemistry

Code: 106044
ECTS Credits: 9

Degree	Type	Year	Semester
2500897 Chemical Engineering	FB	2	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: No
Some groups entirely in Spanish: No

Teachers

Josep Sauri Jimenez

Prerequisites

It is very convenient for the student to review the general concepts acquired in the first year with the subject of Inorganic Chemistry and Equilibrium. In particular, the part that refers to chemical and acid-base balance. A minimum knowledge of organic formulation and nomenclature is required.

Remember that this is a subject where part of the assessment can be carried out during class (theory and / or problems). For this reason, it is highly recommended when enrolling, to consider possible overlaps with scheduled activities of other subjects.

Objectives and Contextualisation

The student should be able to identify the main functional groups and their corresponding oxidation degrees.

The student should be able to acquire a basic structural knowledge of organic molecules and organic stereochemistry.

The student should be able to identifie the possible synthetic precursors of the main functional groups as well as to have a basic knowledge of their reactivity.

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.
- 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.

Learning Outcomes

1. Associate the properties and reactivity of the main families of bioorganic compounds with the functional groups that they contain.
2. Be able to classify organic compounds and recognise reactivity from the functional groups that are present.
3. Identify simple organic compounds from the spectroscopic and analytical properties of their functional groups and relate the structural characteristics with their physical and chemical properties.
4. Propose effective synthetic pathways for the preparation of simple organic compounds and evaluate synthesis processes of simple organic compounds using criteria of energetic and atomic economics (green chemistry).
5. 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.
6. Understand the concept of stereoisomerism and be able to identify the type and number of stereoisomers in a certain organic compounds.
7. Understand the essential principles of the stability and reactivity of organic compounds.

Content

1. Introduction. Basic Concepts in Organic Chemistry

Chemical bond. Lewis structures and resonance. Atomic orbitals, hybrid orbitals and molecular orbitals. Polarity. Intermolecular forces. Structures and formulas of organic molecules. Oxidation degree. Classification of compounds according to the degree of oxidation and their functional group. Thermodynamics and equilibrium. Kinetics and reaction mechanisms: elementary and multistep reactions, reaction coordinate and profile, transition state, reaction intermediates, catalysis. Organic nomenclature. Acids and Bases in Organic Chemistry.

2. Stereochemistry

Isomerism. Chirality. Stereogenic center. *R*/*S* nomenclature. Enantiomers and diastereomers. Racemic mixture. *Meso* forms. Fischer projections. Optical activity, optical purity. Isomerism of *cis-trans* alkenes (*Z*/*E*). Chiral molecules and their biological importance.

3. Alkanes

Classes of alkanes: homologous series. Physical properties. Sources for obtaining alkanes, oil fractional distillation. Alkane halogenation reactions: Homolytic and heterolytic bond breaking, chain reactions and reactivity / selectivity.

4. Alkenes and alkynes

Physical properties. Sources of obtaining alkenes: cracking of naphtha. Obtaining alkenes by elimination. Hydrogenation reactions of alkenes. Alkene addition reactions. Isomerization of alkenes. Polymerization of alkenes. Alkene oxidation reactions. General reactivity of alkynes.

5. Aromatic compounds

Benzene: electronic structure. Resonance. Aromaticity criteria. Aromatic electrophilic substitution reactions (S_EAr): Effects of substituents on S_EAr, reactivity and orientation.

6. Compounds with Degree of oxidation = 1

Alkyl halides, alcohols, ethers, amines, thiols, thioethers. Concepts: Nucleophile and electrophile. Nucleophilic substitution reactions (S_N1-S_N2 mechanisms). Elimination reactions (mechanisms *E*1-*E*2). Basicity and nucleophilicity.

7. Compounds with Degree of oxidation = 2

Aldehydes and ketones. Structure and reactivity of the carbonyl group. Obtention reactions. Oxidation and reduction reactions. Nucleophilic addition reactions. Acetals and hemiacetals. Carbohydrates. Schiff Bases. Aldolic condensation.

8. Compounds with Degree of oxidation = 3 and 4

Carboxylic acids and derivatives. Urethanes and carbamates. Acid structure and character. Obtaining reactions. Interconversion reactions of carboxylic acids and their derivatives: acid halides, anhydrides, esters, amides. Amino acids, peptides and proteins. Carboxylic acids and derivatives of industrial interest: synthetic fibers, lipids and natural fats. Urethanes and carbamates.

Methodology

In accordance with the objectives of the subject, in the course of the semester, the student must be involved in a series of activities to achieve the established objectives.

In general, teaching activities can be grouped into three different types:

Theoretical classes: In this case, students receive a series of knowledge articulated exclusively by the Professor. It is intended that this scientific-technical knowledge will serve as a basis for further maturation by students. In any case, as far as possible, student participation will be encouraged through the dynamization of classes by resolving cases and questions on a regular basis.

Problem solving classes: At the beginning of each lesson, students will have a collection of problems with which students will put into practice, the knowledge acquired in the Theory classes and the tasks that derive from 'these. The problem classes will focus on solving all the problems that the fixed time allows. Special emphasis will be placed on the active participation of students in solving the problems that arise as well as proposed exercises. These exercises, in some cases, could be proposed in such a way that through the solutions proposed by the students, the objectives to be achieved can be evaluated.

Seminars: Throughout the course there will be sessions dedicated to clarifying doubts and / or correcting assessment tests.

Practice sessions: There will be practice sessions in the laboratory related to the contents of the theoretical classes and the problem-solving classes. Attendance is mandatory at all sessions.

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			
Laboratory Practice Sessions	35	1.4	1, 7, 3, 5, 2
Seminars	6	0.24	1, 6, 7, 3, 4, 2
Solving Problems classes	18	0.72	1, 6, 7, 3, 4, 5, 2
Theory lectures	38	1.52	1, 6, 7, 3, 4
Type: Autonomous			
Problem Solving	34	1.36	1, 6, 7, 3, 4, 5, 2
Study and expansion of the concepts explained in the classroom	83	3.32	1, 6, 7, 3, 4, 5, 2

Assessment

1. General

The assessment regulations are shown below. In addition, on the first day of class (Theory) there will be an explanation of the procedures of the subject where emphasis will be placed on the evaluation of the subject.

In this subject, the scientific-technical knowledge of the subject acquired by the student is evaluated individually, as well as its capacity of analysis, synthesis and critical reasoning. The overall grade of the subject will be calculated based on 3 grades, each with a different contribution:

Part 1: Exams (60% contribution to the total course).

Part 2: Exercises (15% contribution to the total course).

Part 3: Internships (25% contribution to the total course).

Each of the parts is detailed below:

2. Parts in which the global evaluation of the subject is divided

2.1. Part 1: Exams (60%):

2.1.1. Partial exams (60%):

Two written partial exams: The assessed subject will include all that is taught until the date of the test (1st part) and from the resumption of classes after the 1st part until the date of the part (2nd part). The mark obtained in the 1st part contributes 30% and that of the 2nd 30% both on the overall mark of the subject.

2.2.2. Final test (recovery) (60%):

The assessed subject will include all that is taught during the course. This test has two purposes:

a) Anyone who has not passed the course with the partial exams must present to pass the course. The grade obtained will be equivalent to the average of the two partials and will contribute 60% to the final grade of the subject.

b) Any student who has passed the course in part may present to raise the grade of Part 1 (Exams). You will be able to take the exam and decide at the end of the exam time whether to deliver or not. In case of delivery, the mark that will finally count as Part 1 will be that of the final exam. If it does not deliver, the mark will be the one obtained by average of the partial ones.

2.2. Part 2: Exercises (15%):

Throughout the course, a number of short, quick-answer questions will be proposed and collected. These exercises can be proposed in both Theory and Problem Solving classes. The number of questions to evaluate is not predetermined. The mark of these tests will contribute 15% to the final mark. Failure to present one of these exercises will be counted as 0.0 points when averaging to calculate the grade for Part 2.

2.3. Part 3: Internship grade (25%):

The practice sessions will have a weight of 25% on the final mark of the subject. This percentage will be divided into: 10% of attitude and results in the laboratory (this grade will not be recoverable), 15% of a written exam that will be done at the end of the laboratory sessions. Attendance at laboratory sessions is mandatory and in no case may be less than 80% to pass the course. Any omission must be justified to the professor responsible for the laboratory. Failure to comply with the safety rules in the laboratory will mean the immediate expulsion of the same and therefore the loss of the right to be evaluated of the practices with which it will not have the possibility of passing the subject.

3. Global Qualification of the Subject

We define:

3.1. Student who PASSES the subject

3.1.1. Students who pass the subject will only be considered those who meet the following 2 sections a and b:

a) That they have obtained at least 4 out of 10 points in each of the partial exams and also have a

average equal to or greater than 5 points out of 10 (Part 1). Alternatively, if you take the final exam, your mark will be 5 out of 10 or higher.

b) That they have a mark of practices (Part 3) equal or upper to 5 out of 10. The mark of the written examination of practices has to be at least of 4.

There is no minimum grade with respect to Part 2 (exercises performed in class) the grade that is average of the sum of the grades of the exercises presented with respect to the total of the exercises proposed throughout the course, will be applied contributing 15% of the grade of the subject.

3.1.2. Honor Rolls. For each subject of the same curriculum, the honors enrollments resulting from calculating the five percent or fraction of the students enrolled in all the teaching groups of the subject will be granted globally. They can only be awarded to students who have obtained a final and overall grade of the subject equal to or greater than 9.00.

3.1.3. VERY IMPORTANT:

For students enrolled for the second time or more:

If the student wishes, it will not be necessary for him to carry out the practices and the note of practices obtained in the course where he carried them out will be counted. In any case, if the student wants to repeat the internship, the grade obtained in this course will be applied.

3.2. Student who does NOT PASS the subject

Any student who does not meet any of the conditions mentioned in section 3.1.1. The note that will appear in your file will be the one that results from applying the weighting between the different Parties mentioned in section 2.

3.3. Student with a grade of NON-EVALUABLE.

Non-Evaluable students will be considered those who:

a) If they are enrolled for the 1st time: They have not taken any of the written assessment tests (Part 1) or the internships.

b) If they are enrolled 2 or more times: They have not taken any of the written assessment tests (Part 1).

4. IRREGULARITIES:

Without prejudice to other disciplinary measures deemed appropriate, and in accordance with current academic regulations, any irregularities committed by the student that may lead to a variation in the qualification of an act of evaluation. Therefore, copying or copying a practice or any other assessment activity will involve failing it with a mark=0, and if it is a condition to pass the whole subject, the whole subject will be failed. Assessment activities qualified in this way will not be recoverable and therefore the subject will be failed directly without the opportunity to recover it in the same academic year.

5. Communication

The main communication tool to disseminate the materials of the subject, lists of notes and news will be the virtual platform Moodle (*Campus Virtual*).

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
2 midterm exams	60%	6	0.24	1, 6, 7, 3, 4, 2
Deliverable Exercices	15%	0	0	1, 6, 7, 3, 4, 5, 2
Laboratory Practices Exam	25%	2	0.08	1, 6, 7, 3, 4, 2
Retake Exam	60%	3	0.12	1, 6, 7, 3, 4, 2

Bibliography

P.Y. Bruice. Organic Chemistry (6th Ed.) Prentice-Hall International - Pearson Education, 2010.
F.A. Carey. Organic Chemistry (8th Ed.) McGraw-Hill, 2011.
T.W.G. Solomons. Organic Chemistry (9th Ed.), Wiley Publishing, New York, 2008.
K.P.C. Vollhardt; N.E. Schore Química Orgánica. Estructura y Función (5ª Ed.), Omega, 2008.
W.R. Peterson. Formulación y nomenclatura en Química Orgánica, EUNIBAR, 1987.

Software

Nomenclature and Structures:
http://www.freechemsketch.com/