Structure and Reactivity of Organic Compounds

Code: 102528
ECTS Credits: 12

2024/2025

Degree	Type	Year
2502444 Chemistry	OB	2

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

It is necessary to have pass the following subjects of the 1st course of the Chemistry Degree:

Fonaments de Química I

Experimentació i Recursos Informàtics

Objectives and Contextualisation

The proposed program aims to provide an overview of organic compounds, both from the structural point of view and their reactivity. In general terms, the subject is organized based on the common and differential reactivity of the various functional groups. The stereochemical aspects of organic molecules will also be studied.

The specific objectives are:

1. Study of the conformational and stereochemical analysis of organic molecules.
2. Study of the structure and reactivity of the main functional groups.
3. Study of synthetic methodologies for the formation of carbon-carbon bonds and interconversion of functional

groups.
4. Introduction to the mechanisms of organic reactions.
5. Learning of basic experimental techniques and procedures of an Organic Chemistry laboratory.

Competences

- "Interpret data obtained by means of experimental measures, including the use of IT tools; identify their meaning and relate the data with appropriate chemistry, physics or biology theories."
- Adapt to new situations.
- Apply knowledge of chemistry to problem solving of a quantitative or qualitative nature in familiar and professional fields.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Evaluate the health risks and environmental and socioeconomic impact associated to chemical substances and the chemistry industry.
- Handle chemical products safely.
- Handle standard instruments and material in analytic and synthetic chemical laboratories.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Obtain information, including by digital means.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Show sensitivity for environmental issues.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.
- Work in a team and show concern for interpersonal relations at work.

Learning Outcomes

1. Adapt to new situations.
2. Apply the acquired theoretical contents to the explanation of experimental phenomena.
3. Be ethically committed.
4. Carry out basic synthesis, separation and purification procedures in an organic chemistry laboratory.
5. Communicate orally and in writing in one's own language.
6. Critically evaluate experimental results and deduce their meaning.
7. Describe the different types of isomerism in organic compounds.
8. Describe the mechanisms of the principal organic reactions and the various factors that affect them.
9. Describe the most relevant synthetic methodologies for the inter-conversion of functional groups and the formation of simple and multiple carbon-carbon bonds.
10. Determine and represent the configuration of chiral centres in organic compounds.
11. Have numerical calculation skills.
12. Identify the basic reactivity associated with the various functional organic groups.
13. Identify the functional groups of the principal natural organic products and their most important reactions.
14. Identify the isometric relationship between different structures of organic compounds.
15. Identify the risks in the handling of organic chemical compounds in the laboratory, and apply the suitable protocols for the storage or elimination of the waste generated.

16. Justify the results obtained in the laboratory for the processes of synthesis, separation, purification and characterisation of organic compounds.
17. Learn autonomously.
18. Manage the organisation and planning of tasks.
19. Manage, analyse and synthesise information.
20. Obtain information, including by digital means.
21. Predict the reactivity of different organic functional groups under certain reaction conditions, as well as the structure of the products obtained.
22. Properly handle glass and other common materials in an organic chemistry laboratory.
23. Propose creative ideas and solutions.
24. Propose reaction mechanisms in processes involving organic compounds.
25. Propose simple synthetic methods to obtain certain organic compounds from certain reagents.
26. Reason in a critical manner
27. Recognise the English names of the basic materials and instruments in an organic chemistry laboratory.
28. Resolve organic chemistry problems with the help of the provided complementary bibliography.
29. Resolve problems and make decisions.
30. Safely manipulate chemical reagents and organic compounds.
31. Show initiative and an enterprising spirit.
32. Show motivation for quality.
33. Show sensitivity for environmental issues.
34. Use IT to treat and present information.
35. Use basic instruments to characterise organic chemical compounds.
36. Work in a team and show concern for interpersonal relations at work.

Content

1. Introduction. Basic concepts in Organic Chemistry

Atomic orbitals, hybridization, molecular orbitals and chemical bonding in organic molecules. Geometry in organic molecules.

Lewis structures and resonant forms.

Oxidation degree and oxidation state.

Classification of compounds according to the oxidation degree. Functional groups.

Thermodynamics and equilibrium, basic concepts in organic reactivity. Enthalpy, entropy and Gibbs free energy.

Reaction kinetics and mechanisms: elementary reaction and steps of a mechanism, reaction coordinate and profile, transition state, reaction intermediates, catalysis. Eyring equations (free enthalpy of activation) and Arrhenius (free energy of activation).

Organic Nomenclature.

2. Conformational and stereochemical analysis

Introduction to organic compounds. Structural or constitutional isomerism.

Conformational isomerism: representation through Newman and cavalier projections.

Conformational analysis of alkanes.

Cycloalkane: ring strain.

Conformational analysis of cyclohexane. Conformational balance in substituted cyclohexanes.

Configuration isomerism cis-trans on cycles.

Configuration isomerism Z-E of alquens.

Enantioisomers and diastereoisomers. Chirality.

Configurational isomerism in compounds with stereogenic centers: representation and nomenclature *R*/*S*.

Optical activity: optical rotation and optical purity.

Configurational isomers with more than one stereogenic center: *meso* forms.

Racemic mixtures Resolution of racemates.

3. Radical substitution reactions

Halogenation of alkanes.

Bond energies, free radicals and relative stability.

Reactivity *versus* selectivity in the halogenation of alkanes. Hammond Postulate.

Radical substitution of allylic, benzylic and arylic hydrogens.

4. Nucleophilic substitution on saturated carbons

S_N1 and S_N2 reactions: mechanisms and stereochemistry.

Leaving groups. Alkyl halides, alcohols and ethers. Effect on the reactivity and activation of the nucleophug.

Nucleophils: acetylur and cyanide; water, alcohols and thiols; ammonia, amines and imides. Effect on the reactivity.

Other aspects that influence the reactivity.

Competition between S_N1 and S_N2.

5. Elimination reactions

E1 and E2 reactions for the formation of carbon-carbon multiple bonds: mechanisms

Leaving groups, substrates and bases in reactions E1 and E2. Dehydration of alcohols.

Regioselectivity in reactions E1 and E2. Zaitsev rule and stability of alkenes.

Stereochemistry of the E1 and E2 reactions.

Competition among S_N1, S_N2, E1 and E2.

Oxidation of alcohols.

6. Addition to multiple carbon-carbon bonds

Electrophilic addition to alkene and alkynes: general mechanism.

Addition of hydrogen halides to alkenes. Cationic intermediates: Markovnikov rule.

Addition of water and alcohols to alkenes. Carbocation rearrangements.

Oximercuration-demercuration and hydroboration.

Addition of halogens to alkenes.

Addition of hydrogen to alkenes.

Polymerization of alkenes.

Addition reactions to alkynes.

Conjugated, isolated and accumulated diens. Relative stability.

Electrophilic addition to conjugated diens: 1,2- *versus* 1,4-addition; kinetic *versus*thermodynamic control.

7. Nucleophilic addition to the carbonyl group

Reactivity of the carbonyl group. Nucleophilic addition mechanisms.

Addition of carbon nucleophiles: cyanide and acetylure compounds and organometallic compounds.

Addition of nitrogen nucleophiles.

Addition of oxygen nucleophiles.

Addition of sulfur nucleophiles.

Addition of hydrides: reduction of aldehydes and ketones.

8. Nucleophilic substitution in the acyl group

Acyl transfer reactions of carboxylic acids and derivatives: addition-elimination mechanism and the effect of the leaving and nucleophile groups. Interconversion reactions: formation and hydrolysis of carboxylic acid derivatives.

Reduction of acids and derivatives.

Reactions with organometallic compounds.

Derivatives of phosphoric acid.

Condensation polymers: functional groups of 4th degree of oxidation.

9. Reactivity of alpha carbon in carbonyl systems

Acidity of the hydrogens in the alpha carbon. Effect on the reactivity.

Keto and enol tautomers.

Alpha-halogenation of aldehydes and ketones. Alpha-halogenation of carboxylic acids.

Formation of alpha,beta-unsaturated carbonyl compounds: aldol condensation.

Cannizzaro reaction.

Formation of beta-dicarbonyl compounds: Claisen and Dieckmann condensations.

Beta-dicarbonyl compounds: acetoacetic and malonic synthesis.

10. Substitution reactions in aromatic compounds

Aromatic compounds: benzene, polycyclic and heterocyclic.

Reaction with electrophiles: aromatic electrophilic substitution (S_EAr).

S_EAr in benzene: nitration, sulfonation, halogenation, Friedel-Crafts acylation and Friedel-Crafts alkylation.

S_EAr in substituted benzenes: effect on reactivity and orientation.

Diazonium salts. Copulation reactions.

Reaction with nucleophiles: aromatic nucleophilic substitution (S_NAr), addition-elimination mechanism.

Substituted benzenes from diazonium salts.

Substitution reactions in heterocyclic aromatic compounds.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Laboratory practices	48	1.92	1, 4, 5, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 26, 27, 29, 30, 31, 32, 33, 35, 36
Problem classes	20	0.8	1, 5, 7, 8, 9, 10, 11, 12, 13, 14, 17, 19, 20, 21, 23, 24, 25, 26, 29, 34, 36
Seminaires	4	0.16	2, 5, 6, 7, 8, 9, 10, 12, 13, 14, 18, 19, 21, 24, 25, 28, 29
Theoretical classes	58	2.32	1, 3, 5, 7, 8, 9, 10, 12, 13, 14, 17, 19, 20, 21, 24, 25, 26, 33
Type: Autonomous			

Study, problems resolution, practices preparation	158	6.32

The Virtual Campus will be used to deliver to students all the materials that the professors consider necessary for the learning process: subject program, presentations of the syllabus, problems to be solved, linking the content to be developed with various proposed textbooks, etc.

Students in continuous evaluation and single evaluation modality:

In accordance with the objectives of the subject, students throughout the academic year must be involved in a series of training activities aimed at achieving the established knowledge and skills. These activities will be:

In-person lectures: During part of these in-person sessions the teaching staff will highlight selected theoretical aspects of the subject of the different topics. Another part of these classes will be presented as seminars, dedicating time to resolving students' doubts, both regarding theoretical content or problems and organizational issues of the course.

In-person problem-solving classes: In these sessions, solutions proposed by teachers or students will be presented and discussed, based on autonomous work developed individually or in groups, for previously posed problems. Special emphasis will be placed on the active participation of students.

Laboratory practices: 12 laboratory sessions (4-hour each) will be carried out to guarantee the acquisition of the basic techniques of an organic synthesis laboratory. The contents of these sessions will be linked to the topics covered in the previous theoretical class period. Attendance at all 12 sessions is mandatory. A laboratory presentation session is scheduled, which is also mandatory attendance.

Note: In the in-person lectures, a series of evaluative tests (evidence) will also be carried out throughout the course. On a regular basis, student participation will be encouraged by solving cases and questions. These evaluation activities will not be mandatory for these students in a single evaluation modality.

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.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evaluation of laboratory practices	15%	2	0.08	1, 2, 3, 4, 5, 6, 11, 15, 16, 17, 18, 19, 20, 22, 23, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36
Other evidences	10%	0	0	5, 7, 8, 9, 10, 12, 13, 14, 17, 19, 20, 21, 23, 24, 25, 26, 28, 29, 34, 36
Partial and recovery exams	75%	10	0.4	2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 15, 16, 21, 23, 24, 25, 26, 27, 29, 30

1. ASSESSMENT

1.1. Students with Continuous Evaluation modality:

The final overall grade for this subject is calculated from the grades obtained in the following 3 parts:

1.1.1. Exams (75% of the final grade): The exams will evaluate the knowledge contained in the subject program, with special emphasis on the ability to solve problems.

During the course, each midterm will include questions about the entire syllabus taught so far. These exams will have an increasing specific weight on the total final grade of the exams:

- First partial: Chapters 1 to 4; incidence on the final grade of 20%.

- Second partial: Chapters 1 to 7; incidence on the final grade of 25%.

- Third partial: Chapters 1 to 10; incidence on the final grade of 30%.

To pass the subject by midterm exams, a minimum grade of 4 points out of 10 will be required in the third midterm exam and 5 points out of 10 for the weighted average of the 3 partial exams.

1.1.2. Laboratory practices (15% of the final grade): Interest, experimental ability and the results obtained during the laboratory sessions (40%) will be valued, as well as the grade obtained in the practical exam (60%). Practice sessions are mandatory. A maximum of two sessions may be missed in case of medically justified illness. To average and to pass the laboratory practices, there will be a minimum grade of 5 points out of 10 both in the grade for the laboratory sessions and in the grade for the practical exam (ordinary call). If you obtain a grade of less than 5 points out of 10 in the exam, you must attend a retake of the practice exam on the same day as the retake of the Theory part of the subject. In order to be able to take the practice retake exam, it is essential to have taken the practice exam in the ordinary session.

WARNING ABOUT SAFETY IN THE LABORATORY: The person who, as a result of negligent behavior, is involved in an incident that may have serious safety consequences may be excluded from the laboratory and fail the subject.

Students enrolled for the 2nd or more time, who in a previous course carried out the laboratory practices in compliance with the conditions established for their approval, may not repeat them and the grade from the previous course will be maintained.

1.1.3. Other evidence (10% of the final grade): Throughout the course, exercises, questionnaires or other small tasks may be proposed to be carried out individually or in groups, in class or outside of class at the discretion of the teaching staff. Evidence not carried out will count as 0.0 out of 10 when calculating the average.

1.2. Students with Single Evaluation modality:

The final overall grade for this subject is calculated from the grades obtained in the following 2 parts:

1.2.1. Final Exam (85% of the final grade): The exam will evaluate the knowledge contained in the subject program, with special emphasis on the ability to solve problems. The exam will be scheduled on the same day that the students who opt for the continuous evaluation route take the third partial.

1.2.2. Laboratory practices (15% of the final grade): The same conditions apply as to students in continuous evaluation mode.

2.2. Students with Single Evaluation modality:

2.2.1. Conditions

a) - To obtain a grade in the global exam of the subject of 5 points out of 10 or higher.

b) - To have completed all the practice sessions and obtained a minimum grade of 5 points out of 10 in their overall evaluation and a minimum grade of 5 points out of 10 in both parts that are averaged by the calculation of the overall practice grade.

c) - Obtain a global average of all evaluable aspects of 5 out of 10 points.

2.2.2. Retake:

There will be a single retake exam for students who opt for the single evaluation modality. The exam will be scheduled on the same day as the retake exam for students who opt for continuous assessment.

Students who have passed the course and want to improve their grade may take the retake exam. In this case, if the exam is submitted answered, in all cases, the grade obtained will replace the weighted average of the midterms. If you do not submit it, you will retain the grade of the weighted average previously obtained.

This exam will include material from the entire course.

In order to pass the subject, students will have to obtain a minimum grade of 5 points out of 10 in the retake exam. The final grade for the subject, if you have participated in the retake exam, will consist of two parts:

85% grade of the retake exam.

15% final grade for laboratory practices.

3. STUDENTS WILL BE CONSIDERED NOT EVALUABLE THOSE WHO:

a) If you are enrolled for the 1st time and opt for the continuous evaluation route: You have not taken any of the partial exams or the practices.

b) If you are enrolled for the 2nd time or more, have the practices approved and opt for the continuous evaluation route: You have not taken any of the partial exams or the practices in the current course.

c) If you are enrolled for the 1st time and opt for the single evaluation route: You have not taken the final exam or the practices.

d) If you are enrolled for the 2nd time or more, have the practices approved and opt for the single evaluation route: You have not taken the final exam or the practices in the current course.

IMPORTANT NOTICE: Students who are found to have cheated in any of the evaluation tests will have a 0 as a grade for the corresponding test.

Bibliography

Text books:

Organized by reactivity: Joseph M. Hornback, *Organic Chemistry*, Ed. Thomson Brooks/Cole, 2006

Organized by functional groups:

K.P.C. Vollhardt; N.E. Schore, *Organic Chemistry: Structure and Function (8th Ed)*, Ed. McMillan Learning 2018; K.P.C. Vollhardt; N.E. Schore, *Organic Chemistry* (*6th Ed.*), Ed. Freeman, WH & Company, 2009; K.P.C. Vollhardt; N.E. Schore, *Química Orgánica. Estructura y Función (5ª Ed.)*, Ed. Omega, 2008.;

P. Y. Bruice, *Organic Chemistry*, (*8th Ed.*); University of California, Santa Barbara, Pearson, 2017.

This book is available in electronic format: https://cataleg.uab.cat/iii/encore/record/C__Rb2084284?lang=cat

Nomenclature in Spanish: W.R. Peterson. *Formulación y nomenclatura en Química Orgánica*, EUNIBAR, 1987.

Websites:

Terms of chemistry dictionary: http://goldbook.iupac.org/

Organic Chemistry Portal:www.organic-chemistry.org

Virtual site of the subject: Moodle

Degree in Chemistry Website:
https://www.uab.cat/web/estudiar/llistat-de-graus/informacio-general/quimica-1216708251447.html?param1=126

Software

Free software Molecular structure drawing, nomenclature:

http://www.freechemsketch.com/

https://chemaxon.com/products/marvin

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	annual	morning-mixed
(PAUL) Classroom practices	2	Catalan	annual	morning-mixed
(PLAB) Practical laboratories	1	Catalan/Spanish	annual	morning-mixed
(PLAB) Practical laboratories	2	Catalan	annual	morning-mixed
(PLAB) Practical laboratories	3	Catalan/Spanish	annual	afternoon
(PLAB) Practical laboratories	4	Catalan	annual	afternoon
(SEM) Seminars	1	Catalan/Spanish	annual	morning-mixed
(SEM) Seminars	2	Catalan/Spanish	annual	morning-mixed
(TE) Theory	1	Catalan	annual	morning-mixed
(TE) Theory	2	Catalan	annual	morning-mixed