Universitat Autònoma de Barcelona

2022/2023

Structure and Reactivity of Organic Compounds

Code: 102528
ECTS Credits: 12

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	A

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

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Prerequisites

It is necessary to have pass the following subjects of the 1st course of the Chemistry Degree: *Fonaments de Química I 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. 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.

2. 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.

3. 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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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.

9. 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.

Methodology

The *Campus Virtual* will be used to deliver to the students all the resources that the teachers consider necessary for the learning process: syllabus of the subject, presentations of the syllabus, problems to solve, linking the content to be developed with several proposed textbooks, etc.

In accordance with the objectives of the course, students must be involved in a series of targeted training activities during the year in order to achieve the established knowledge and skills. These activities will be:

Lectures: During a part of these face-to-face sessions, teachers will highlight selected theoretical aspects of the subject of the different topics. Another part of these classes will be presented as seminars, devoting time to resolving students' doubts, both about theoretical content or problems and about organizational issues of the course. Finally, in these classes there will also be a series of small assessment tests (evidences) throughout the course. Student participation will be encouraged by resolving cases and questions on a regular basis.

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

Laboratory Practices: A series of 4-hour laboratory sessions will be conducted to ensure 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.

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 practices	48	1.92	1, 17, 5, 31, 32, 4, 18, 19, 13, 15, 12, 14, 16, 22, 30, 33, 20, 21, 23, 26, 27, 29, 11, 36, 35
Problem classes	20	0.8	1, 17, 5, 7, 8, 9, 10, 19, 13, 12, 14, 20, 21, 23, 24, 25, 26, 29, 11, 36, 34
Seminaires	4	0.16	2, 6, 5, 7, 8, 9, 10, 18, 19, 13, 12, 14, 21, 24, 25, 28, 29
Theoretical classes	58	2.32	1, 17, 5, 7, 8, 9, 10, 19, 13, 12, 14, 3, 33, 20, 21, 24, 25, 26
Type: Autonomous			
Study, problems resolution, practices preparation	158	6.32	

Assessment

The final global mark for this course is calculated from the grades obtained in the following 3 parts:

Exams (75% of the final mark): In the exams, the knowledge contained in the subject program will be evaluated, with special emphasis on the ability to solve problems.

There will be three Midterm exams of a maximum duration of three hours. During the course, each Midterm will include questions about all the topics taught since the beginning of the course. These exams will have an increasing specific weight on the global mark corresponding to the contribution of exams part:

- First part: lessons from 1 to 3; impact on the final mark of 20%.

- Second part: lessons from 1 to 6; impact on the final mark of 25%.

- Third part: lessons from 1 to 9; impact on the final mark of 30%.

In order to have a weighted average to pass the course by Midterm exams, a minimum mark of 5 points out of 10 must be obtained in the third Midterm.

Laboratory practices (15% of the final mark): The interest, the experimental ability and the results obtained during the laboratory sessions (40%), as well as the grade obtained in the practice exam (60%) will be valued. Practice sessions are mandatory. A maximum of two sessions may be missed in case of medically justified illness. To average to pass the laboratory practices, you must have a minimum mark of 5 points out of 10 both in the the laboratory sessions mark and in the practice exam mark.

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

The student enrolled for the 2nd time or more, who in a previous course carried out the laboratory practices in person and fulfilling the conditions established to pass them, may not repeat them and the grade from the previous course will be maintained. Students who have never done the face-to-face practices will have to do them and will be evaluated following the same procedure as students enrolled for the first time.

Other evidences (10%): 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. The tests not carried out will compute with a 0.0 out of 10 when calculating the average.

To pass the subject by course it is necessary:

a) - To obtain a weighted average mark of 5 points out of 10 or higher for the three Midterm exams and a minimum mark of 5 out of 10 in the third Midterm exam. Students who have taken the Make-up exam must have obtained a minimum mark of 5 points out of 10.

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

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

Retake:

There will be a single Make-up exam for all students who have not passed by Midterm exams. Students who have passed the Midterm exams and want to improve their mark can also take the Make-up exam. If they deliver it, in all cases, the mark they obtain will replace the weighted average of the Midterm exams. If they do not deliver it, they will keep the mark of the weighted average previously obtained.

To participate in the Make-up exam of the theoretical part, students must have taken the three Midterm exams of the subject.

This exam will include materials concerning the entire course.

In order to pass the subject, students who have not passed the partial exams will have to obtain a minimum grade of 5 points out of 10 in the Make-up exam. The final mark of the subject, if you have participated in the Make-up exam, will consist of three parts:

75% mark of the make-up exam.

10% evaluation through evidence.

15% final mark of laboratory practices.

NON-ASSESSABLE students will be considered those who:

a) If being enrolled for the 1st time: You have not taken any of the Midterm exams or Laboratory Practices.

b) If being enrolled for the 2nd time or more and having passed the Laboratory Practices: You have not taken any of the Midterm exams or not done the Laboratory Practices.

IMPORTANT WARNING: Students who are found to have cheated in any of the tests carried out during the continuous assessment will have a 0 as the mark for the corresponding test.

Assessment Activities

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

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