Universitat Autònoma de Barcelona

2023/2024

Structure and Reactivity of Organic Compounds

Code: 102528
ECTS Credits: 12

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	A

Contact

Name: Juan Pablo Bayon Rueda

Email: pau.bayon@uab.cat

Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject.
Please note that this information is provisional until 30 November 2023.

Teachers

Marta Figueredo Galimany

Roser Pleixats Rovira

Juan Pablo Bayon Rueda

Ona Illa Soler

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.

Methodology

The *Campus Virtual* will be used to provide students with all the materials that the teaching staff deems necessary for the learning process: subject program, syllabus presentations, problems to be solved, linking the content to be developed with various textbooks proposed, etc.

Student in continuous assessment and single assessment modality:

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

Face-to-face master classes: During part of these face-to-face sessions, the teaching staff will highlight selected theoretical aspects of the subject. Another part of these classes will be set up as seminars, devoting time to solving students' doubts, both regarding theoretical content or problems and organizational issues of the course.

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

Laboratory practices: 12 laboratory sessions (4-hour each) will be held in order to ensure the acquisition of the basic techniques of an organic synthesis laboratory. The contents of these sessions will be linked to the topics discussed in the previous theoretical class period.

Note: In face-to-face master classes, a series of assessment tests (evidence) will also be carried out throughout the course. As usual, student participation will be encouraged through the resolution of cases and questions. These assessment activities will not be mandatory for those students in the single assessment 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.

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

1. Assessment

1.1. Student with Continuous Assessment modality:

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

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

Throughout the course, each mid-term exam will include questions on all the syllabus taught so far. These mid-term exams will have an increasing specific weight on the total final mark of the Exams contribution:

- First mid-term: topics from lesson 1 to 4; impact on the final mark of 20%.

- Second mid-term: topics from lesson 1 to 7; impact on the final mark of 25%.

- Third mid-term: topics from lesson 1 to 10; impact on the final mark of 30%.

To pass the subject by mid-term exams, the student must have a minimum mark of 4 points out of 10 in the third mid-term exam and 5 points out of 10 in the weighted average of the 3 mid-term exams.

1.1.2. Laboratory practices (15% of the final grade): Interest, experimental skills and the results obtained during the laboratory sessions (40%) will be assessed, as well as the mark obtained in an exam (60%). 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 in both the mark of the laboratory sessions and the mark of the exam. If the student scores a mark of less than 5 points out of 10 in the exam, the student will have to attend a retake of the practical exam on the same day as the retake of the Theory part of the subject.

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

Students enrolled in the subject for the 2nd time or more, who in a previous year carried out the laboratory practices meeting the conditions established to pass them, may not repeat them and the mark of the previous year will be kept.

1.1.3. Other evidences (10% of the final mark): Throughout the course, exercises, quizzes 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 taken will count with a 0.0 out of 10 when calculating the average.

1.2. Student with Single Assessment modality:

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

1.2.1. Final Exam (85% of the final mark): The exam will assess the knowledge contained in the subject's program, with special emphasis on the ability to solve problems.

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

2. TO PASS THIS SUBJECT BY COURSE YOU NEED:

2.1. Student with Continuous Evaluation modality:

2.1.1. conditions

a) - To obtain a weighted average mark of 5 points out of 10 or higher in the three mid-term exams and a minimum scoring of 4 out of 10 in the third mid-term exam. Students who have taken the retake exam must have obtained a retake exam mark of 5 points out of 10 or higher.

b) - To have completed all the Practice sessions and obtained a minimum mark of 5 points out of 10 in their overall assessment and a minimum mark of 5 points out of 10 in both parts that mediate the calculation of the overall practice mark.

c) - To obtain an overall average of all assessable aspects of 5 points out of 10.

2.1.2. Retake:

There will be a single retake exam for all students who have not passed by mid-term exams. This exam will include topics from the entire course.

Students who have passed the course and want to improve their mark can take the retake exam. If they hand it in, in all cases, the mark they get will replace the weighted average of the mid-term exams. If they do not hand it in, they will keep the grade of the previously obtained weighted average.

To participate in the retake exam for the theoretical part, students must have taken at least two of the three partial exams for the subject.

In order to pass the subject, students who have not passed by mid-term exams must obtain a minimum mark of 5 points out of 10 in the retake exam. The final mark of the subject, if you have taken part in the retake exam, will consist of three parts:

75% mark of the retake exam.

10% mark from other evidences.

15% final mark of laboratory Practices.

If a student attends the retake exam to pass the subject and decide not to hand the exam, the final mark will be calculated considering the weighted average of the mid-term exams (if one of the three mid-term exams has not been attended, it will be counted as a 0 for that partial).

There will also be a retake exam for the practice exam for students who did not reach 5 points out of 10 in the practice exam. The part of the mark corresponding to the experimental skill and the results obtained during the laboratory sessions (40%) will not be reassessed.

2.2. Student with Single Assessment modality:

2.2.1. conditions

a) - To obtain a mark in the overall subject exam 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 assessment and a minimum grade of 5 points out of 10 in both parts that mediate the calculation of the overall Practice mark.

c) - Obtain an overall average of all assessable aspects of 5 points out of 10.

2.2.2. Retake:

There will be a single retake exam for students who opt for the single assessment method.

Students who have passed the course and want to improve their mark can take this retake exam. If they hand it in, in all cases, the mark they get will replace the mark of the global exam. If they do not hand it in, they will keep the mark of the global exam previously obtained.

This exam will include the topics of the entire course.

In order to pass the subject, students must obtain a minimum mark of 5 out of 10 in the retake exam. The final mark of the subject, if the student have taken part in the recovery exam, will consist of two parts:

85% grade in the retake exam.

15% final grade of laboratory Practices.

3. THOSE WHO: WILL BE CONSIDERED A NON-ASSESSABLE STUDENT

a) If the student is enrolled for the 1st time and opts for the continuous assessment route: If the student has not taken any of the mid-term exams or the laboratory Practices.

b) If the student is enrolled for the 2nd time or more, having passed the laboratory Practices and opting for the continuous assessment route: You have not taken any of the partial exams or the laboratory Practices in the current year.

c) If the student is enrolled for the 1st time and opts for the single assessment route: If the student has not taken the final exam or the laboratory Practices.

d) If the student is enrolled for the 2nd time or more, having passedthe laboratory Practices and opting for the single assessment route: You have not taken the final exam or the laboratory Practices in the current year.

NOTICE: Students who are found to have cheated in any of the assessment tests will receive a 0 as a grade 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