Universitat Autònoma de Barcelona

2021/2022

Structure and Reactivity of Organic Compounds

Code: 102528
ECTS Credits: 12

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	A

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

Contact

Name: Felix Busqué Sánchez
Email: Felix.Busque@uab.cat

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

Marta Figueredo Galimany
Joan Pau Bayón Rueda
Felix Busqué Sánchez
Ona Illa Soler

Prerequisites

It is mandatory to have approved the following subjects of the 1st course of the Degree of Chemistry: 1) Basics in Chemistry I; 2) Experimentation and Documentations.

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 ones 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 ones 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 provide students with all the material that professors could consider necessary in order to achieve the learning process: program, theoretical expositions, problems to be solved, among others.

Face-to-face classes: during a part of these face-to-face sessions, the teaching staff will highlight selected theoretical aspects of the subject of the different subjects. Another part of these classes will be presented as seminars, dedicating time to answer questions from students, both technical and questions about the methodology and evaluation activities followed. Finally, in these sessions a series of small evaluative tests (evidences) will also be carried out throughout the course. In any case, student participation will be encouraged by solving examples and asking questions on a regular basis.

Face-to-face classes of problems: these sessions will present and discuss proposed solutions by teachers or students, to problems previously raised and on which students have previously worked autonomously. Again, the active participation of students will be promoted.

Professors will allow students to take around 15 minutes in a classroom session to answer the surveys about the teaching development of the professor and the course or module.

el professorat haurà de destinar aproximadament uns 15 minuts d'alguna classe a permetre que el seu alumnat pugui respondre les enquestes d'avaluació de l'actuació docent i d'avaluació de l'assignatura o mòdul.

Non-face-to-face classes: during the course a series of non-face-to-face sessions of guided work will be carried out by the students, based on the material provided through the virtual campus and the indications of the teaching staff. In these sessions some of the evidence may also be scheduled throughout the course.

Laboratory practices: a series of 4-hour laboratory sessions will be carried out in order to guarantee the acquisition of the basic techniques of an organic synthesis laboratory. The contents of these sessions will be linked to the topics developed in the theoretical classes.

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

Exams (75% of the final mark): The exams will assess the knowledge contained in the syllabus of the subject, with special emphasis on the ability to solve problems.

There will be three partial exams lasting a maximum of three hours. Every partial exam will include questions about all the subjects taught so far. These exams will have an increasing contribution over the ponderate averaged final mark of the exams:

- First partial exam (topics of the course 1 to 3, 20% incidence in the final mark)

- Second partial exam (topics of the course 1 to 6, 25% incidence in the final mark)

- Third partial exam (topics of the course 1 to 9, 30% incidence in the final mark)

In order to be able to do the ponderated average of the exams, a 5.0 mark in the third partial exam is needed. In order to be admited to perfom the recovery exam, the average obtained in the partials must be over the 3.5.

Laboratory practice (15% of the final mark): The interest, experimental ability and results obtained during the face-to-face sessions (40%), as well as the grade obtained in the practice exam (60%) will be assessed. Internship sessions are mandatory. A maximum of two sessions may be missed in the event of a medically justified illness. In orde to average both marks, a 5.0 is needed in every part.

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

Students enrolled 2 or more times, who in a previous year will perform the laboratory practices in person and obtain an overall grade in these equal to or greater than 5 points out of 10 may not repeat them and will keep the grade of the previous year. Students who have never done the internships 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 assignments may be proposed to be done individually or in groups, in class or out of class at the discretion of the teachers. The evidences not done will be counted with 0.0 out of 10 when calculating the average.

To pass the subject per course it is necessary:

a) - Have obtained an average mark of the three partial exams of 5 points out of 10 or higher and a minimum grade of 5 points in the thrid partial exam. .
b) - Have completed all the practice sessions and obtained a minimum grade of 5 points out of 10 in their overall assessment.

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

Second-chance exam:

There will be a single retaking exam for all students who have not passed per course. There will be the chance to raise a grade.

To participate in the retaking exam of the theoretical part, students must have taken the three partial exams of the subject.

This exam will include subject matter throughout the course.

Students who have not passed per course must obtain a minimum grade of 5 points out of 10 in the retaking exam. The final mark of the subject if you have participated in the retaking exam will consist of four parts: 75% mark of the retaking exam, 10% continuous assessment and 15% final mark of practices laboratory, and must be 5 points or more out of 10.

Non-EVALUABLE students will be considered those who:

a) If being enrolled for the 1st time: You have not performed any of the partial exams or the practices.

b) If you are enrolled for 2ª times or more and have the internships approved: You have not taken any of the partial exams or the internships.

IMPORTANT NOTICE: Students detected copying in an exam conducted, will have their exam withdrawn and will have a 0 as a grade.

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/

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

ChemDraw: http://sitelicense.cambridgesoft.com/sitelicense.cfm?sid=1111; adreça: xxx@e-campus.uab.es

Organic Chemistry Portal:www.organic-chemistry.org

Virtual site of the subject: Moodle

Software

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