Universitat Autònoma de Barcelona

2019/2020

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 mandatory to have approved the following subjects of the 1st course of the Degree of Chemistry: 1) Basics in Chemistry; 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

In accordance with the objectives of the subject, students during the course would be involved in a series of activities to achieve the established knowledge and competences. These activities can be grouped into three different types:

Master classes: In this case, students receive a series of knowledge exclusively articulated by the teacher. These scientific-technical knowledge is intended to serve as a platform for subsequent maturation by students. In any case, the participation of the student will be usually promoted during classes by means of the resolution of cases and questions.

Problem classes: In these sessions, the solutions proposed by the students will be discussed, based on autonomous work developed individually or in groups, for exercises and problems previously considered. Special emphasis will be given to the active participation of students.

Seminars: Three seminars will be held throughout the course near the partial exams. These sessions will be used to resolve questions about the exam or move on to problems that have not been solved. Students may also propose problems to solve.

Laboratory practices: 12 days of 4h laboratory sessions will be held to learn the basic techniques of an organic synthesis laboratory. The contents of these sessions will be linked to the topics discussed in the previous theoretical classes. There will be a theoretical session of introduction to the practices that will be mandatory (1h).

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	3	0.12	2, 6, 5, 7, 8, 9, 10, 18, 19, 13, 12, 14, 21, 24, 25, 28, 29
Theoretical classes	56	2.24	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	161	6.44	

Assessment

Examinations (69% of the final grade): The exams will evaluate the knowledge contained in the subject's program, with special emphasis on the capacity to solve problems.

There will be three partial exams with a maximum duration of three hours. Each one will have the same

specific weight on the final mark of the examinations part, account for 23%. To make a weigh up of the three eamens, the studentl must obtain a minimum score of 4 points out of 10 in each one of the partial ones. To have the possibility to participate in the recovery exam, all three partial exams must have been previously done.

Laboratory practices (21% of the final mark): Interest, experimental ability and results (40%), as well as the practice test (60%) will be evaluated. The practical sessions are mandatory. Students may not attend a maximum of two sessions due to justified medical reasons. To ponderate with the other practical marks, students must have a minimum score of 5 points out of 10 in the practice exam.

SECURITY WARNING IN THE LABORATORY: The person who is involved in an incident that may have serious consequences of security may be expelled from the laboratory and suspended the subject.

Students enrolled for the 2nd time or more, who in a previous course carried out the laboratory practices and obtained a grade equal to or greater than 5 points out of 10 may not repeat them and the mark will be kept from the previous course.

Students enrolled for the 2nd time or more, who in the previous course passed theoretical part and obtained an score of 5 points out of 10 or higher, may not repeat this part and the grade from the previous course will be maintained.

Other evidences (10%): Throughout the course exercises or other small tasks to do individually or in groups will be planned, in class or out of class according to the teacher's criteria. The works not presented will count with a 0.0 on 10 when calculating the average.

To pass this subject, student must:

a) obtain an average mark of the three partial exams of 5 points over 10 or higher and a minimum score of 4 points in each one of the partial ones. The lower grades will not be compensated by doing the average.

b) complet all the practice sessions and obtain a minimum score of 5 points out of 10 in the final grade and a minimum score of 5 points in the practice exam. The lower grades will not be compensated by doing the average.

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

Recovery:

There will be only one recovery exam for all the students that have not approved by course or those who wish to raise up their note. The students that take the exam to raise the note will have the final mark that goes out of ponder the notes according to the criteria of the recovery (see below). If these students decide to participate in the recovery exams, they must notify this desicion to the corresponding professors.

To participate in the recovery exam, students must have previously done the three partial examinations of the subject (theoretical part).

This exam will include subject matter throughout the course. In addition, this exam will include some questions for the students that have not approved the practical exam that will be assessed separately. To do the average with the other mark of laboratory practices, students must obtain a minimum score of 5 points out of 10 in this part of the exam. No student will be allowed to participate in the recovery exam to raise the mark.

The students that have not approved by course must obtain a minimum score of 5 points out of 10 in the recovery exam, as well as the ones that come to raise note. The final grade of the subject if students have participated in the recovery exam (to approve or to raise note) will consist of four parts: 59% note of the recovery exam, 10% of the average of the note of the three partial examinations, 10% continuous evaluation and 21% final mark of laboratory of practices, and must be 5 points or more on10.

Students that are considered NOT EVALUABLE are those who:

a) If they are enrolled for the 1st time: They have not participated in any of the partial exams or practices.

b) If they are enrolled for a 2nd time or more and have the laboratory practices approved: They have not participated in any of the partial exams or practices.

c) If they are enrolled for the 2nd time or more and have the theory approved: They have not performed any partial exams or practices.

IMPORTANT NOTICE: The students who in some examination of those carried out during the continuous evaluation are copying will be withdrawn the exam and will have a 0 as a note of the corresponding test.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evaluation of laboratory practices	21%	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	69%	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.

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

Teaching and evaluation guides:
https://www.uab.cat/web/estudiar/llistat-de-graus/pla-d-estudis/guies-docents/x-1345467811508.html?param1=1