



IDENTIFYING DATA

Theory of Organic Reactions

Subject	Theory of Organic Reactions			
Code	V11G201V01417			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Optional	4th	2nd
Teaching language	Spanish			
Department				
Coordinator	Vaz Araújo, Belén			
Lecturers	Vaz Araújo, Belén			
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Web				
General description	<p>This subject aims to deepen the knowledge of all aspects related to reactivity in Organic Chemistry and reaction mechanisms. Emphasis will be placed on factors affecting the stabilities of reaction intermediates, chemoselectivity and stereoselectivity. This knowledge will allow students to predict and justify chemical behaviors.</p> <p>English Friendly Program: Foreign students may request from the teaching staff: a) material and bibliographical references in English for the follow-up of the subject; b) attend tutorials in English; c) assessment tests in English.</p>			

Training and Learning Results

Code	
A4	Students can communicate information, ideas, problems and solutions to both specialist and non-specialist audiences
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
B5	Ability to adapt to new situations and to make decisions
C44	Know the main methods for the study of organic reactions mechanisms
D2	Capacity for teamwork
D3	Ability to communicate in both oral and written form in Spanish and / or Galician and / or English

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Understanding the principles and theories related to the main types of chemical reactions and their characteristics.	A4 A5	B5	C44	D3
Knowing the methods of studying the mechanism of an organic reaction.	A4 A5	B5	C44	D3
Knowing the methods to study and propose reaction intermediates.	A4 A5	B5	C44	D3
Rigorously apply the corresponding safety and healthy standards in the laboratory, as well as the proper treatment of the waste generated		B5	C44	D2 D3
Collect data and write in the laboratory notebook, in a clear, concise and rigorous way, the experiments carried out and the conclusions drawn.	A4 A5	B5		D2 D3

Contents

Topic	
1. Thermodynamics and Kinetics of Organic Reactions	Thermodynamic stability. Chemical kinetics. Coordinate diagrams of reaction. Transition state theory. Arrhenius equation. Reaction rate expressions. Kinetic control and thermodynamic control. Hammond's postulate. Curtin-Hammett principle.

2. Methods for the study of Organic Reactions	Applications of chemical kinetics to the study of the mechanisms of reaction. Kinetic isotope effects. Effect of substituents. Hammett correlations.
3. Acid and base catalysis of organic reactions	Acidity and basicity in organic compounds. Specific acid catalysis. General acid catalysis. Basic catalysis.
4. Frontier Orbitals	Fukui postulate. Klopman-Salem Equation.
5. Reaction Intermediates	Radicals. Carbenes. Carbocations. Carbanions. Structure and stability of these intermediates, generation and reactivity. Reaction intermediates detection. Stereochemistry and reaction mechanisms.
Practice 1. Effect of sterics and electronics on the aldol condensation reaction. Hammett correlation.	
Practice 2. Study of the primary isotope effect in the oxidation of 1-phenylethanol	

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	24	36	60
Seminars	11	24	35
Laboratory practical	14	14	28
Problem and/or exercise solving	1	8	9
Presentation	1	4	5
Problem and/or exercise solving	1	12	13

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

	Description
Lecturing	The subject material will be previously provided through the Moovi platform. The teaching staff will present the contents of the subject in a structured manner. Possible doubts arising at the time of the presentation may be clarified during these presentations.
Seminars	The concepts introduced in the master sessions will be worked on through problems and questions formulated by the teaching staff. In addition, the students will work on the concepts learned in class and will solve problems and additional exercises that will be evaluated.
Laboratory practical	The laboratory work will be developed in 4 sessions of 3.5 hours. Students will have to prepare a laboratory notebook with the experiments carried out, where the conclusions derived from the experimental work will also be collected. Additionally, students will answer a series of questions about the work done in the laboratory.

Personalized assistance

Methodologies	Description
Lecturing	The teacher will clarify the doubts and questions that arise during the exposition of the topics, related to the subject.
Seminars	The teaching staff will explain and resolve the questions raised by the students in relation to the exercises and problems solved in the seminar sessions.
Laboratory practical	The teaching staff will supervise and guide the development of the experiments proposed in the lab sessions. In addition, special attention will be paid to compliance with safety and healthy measures in the laboratory.
Tests	Description
Problem and/or exercise solving	Before each evaluation test (short tests and final exam) the teaching staff will dedicate the necessary time to answer the students' questions related to the subject.
Presentation	The teacher will supervise and guide the development of the work for its subsequent presentation in a seminar session.
Problem and/or exercise solving	

Assessment

Description	Qualification	Training and Learning Results

Seminars	As part of the continuous evaluation, the participation and the resolution of the exercises proposed by the teaching staff in the classroom will be evaluated. The resolution of exercises and additional problems will also be evaluated, similar to those resolved during the seminar sessions, and which will be proposed through the Moovi platform.	20	A4 A5	C44	D3
Laboratory practical	1. It is mandatory to carry out the laboratory practices, as well as to follow the healthy and safety standards in the laboratory and the collection of residues to obtain the PASS condition. 2. In addition, it will be evaluated (20%): - the laboratory notebook - the resolution of the questions raised in relation to the practices carried out. 3. In order for students to pass the subject, they must obtain the PASS mark in the laboratory practice work.	20	A5	B5 C44	D2 D3
Problem and/or exercise solving	Two tests will be carried out: The first test on the contents of the first topics, which will mean 20% of the final grade. A minimum grade of 2.5 points out of 10.0 in this test will be required to pass the subject. In the event that the minimum required in any of the tests (first or second) is not exceeded, the final grade obtained in the subject will be the weighted grade of the global evaluation test.	20	A4 A5	B5 C44	D3
Presentation	The students will analyze and explain the research results collected in a recent research article related to the subject of the course in a seminar session. The ability to synthesize and understand the work presented will be valued, as well as the questions that are asked about the other works of the students.	10	A4 A5	B5 C44	D3
Problem and/or exercise solving	Two tests will be carried out: The second test on ALL THE CONTENTS OF THE SUBJECT, which will mean 30% of the final grade. A minimum grade of 4.0 points out of 10.0 in this test will be required to pass the subject. In the event that the minimum required in any of the previous tests is not exceeded, the final grade obtained in the subject will be the weighted grade of the global evaluation test.	30	A4 A5	B5 C44	D3

Other comments on the Evaluation

MINIMUM REQUIREMENTS: The identification of serious conceptual errors will lead to an assignment of specific activities aimed at acquiring those skills. These activities will be evaluated as part of the 20% corresponding to deliverables.

CONDITION OF PRESENTED: The participation of the student in any of the acts of evaluation of the subject will imply the condition of presented and, therefore, the assignment of a grade. Attendance at practical laboratory classes, handing in assignments and/or exercises proposed by the teaching staff, or taking a test will be considered acts of evaluation.

EVALUATION IN JULY: the grade obtained by the students during the course in problem solving, laboratory practices and assignments will be maintained. A test will be carried out on all the theoretical contents of the subject that will account for 45% of the final grade and that will replace the marks of the written tests. It will be necessary to achieve a minimum of 4 points out of 10 in this test to pass the subject and to take into account the rest of the evaluation elements. In case of having a grade of PASS in the laboratory work and having obtained a grade lower than 5 out of 10 in the evaluation of the practices, a written test of the experimental part will be done, which will mean 20% of the final grade.

STUDENTS OF 2nd AND LATER REGISTRATION: Students who have been evaluated with PASS in the laboratory work in a previous course, will be awarded the mention of PASS in the follow-up of the laboratory work in the current academic year, not being necessary to carry out the experiments again. However, a written test of the experimental part must be taken to obtain the qualification corresponding to the experimental part of the subject in the current academic year.

NON-CONTINUOUS ASSESSMENT OPTION: Students who wish not to opt for continuous assessment must request it during the first three weeks of the course from the subject coordinator. To pass the subject, you must complete the Laboratory Practices, obtain a grade of PASS in the work developed in the laboratory and a grade equal to or greater than 5 points out of 10 in the evaluation of the laboratory notebook and the questions related to the practices made. In addition, you must obtain at least 5 points out of 10 in a test in which all the contents of the subject will be evaluated. In this case, the final mark will be a maximum of 2 points for laboratory practices and a maximum of 8 points for the written test.

Sources of information

Basic Bibliography

J. Clayden, N. Greeves, S. Warren., **Organic Chemistry**, Oxford University Press, 2012

Complementary Bibliography

Felix A. Carroll., **Perspectives on Structure and Mechanism in Organic Chemistry**, Wiley, 2010

Francis A. Carey, Richard J. Sundberg, **Advanced Organic Chemistry : Part A: Structure and Mechanisms**, Springer, 2007

Recommendations

Subjects that it is recommended to have taken before

Chemistry: Chemistry Lab I/V11G201V01105

Chemistry: Chemistry Lab II/V11G201V01110

Chemistry: Chemistry 1/V11G201V01104

Chemistry: Chemistry 2/V11G201V01109

Organic chemistry I/V11G201V01205

Organic chemistry II/V11G201V01210

Physical Chemistry V: Chemical Kinetics/V11G201V01308

Organic Chemistry III: Concerted, Radical and Photochemical Reactions/V11G201V01305

Organic Chemistry IV: Design of Organic Synthesis/V11G201V01310
