Universida_{de}Vigo

Subject Guide 2023 / 2024

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IDENTIFYIN	G DATA					
Theory of C	rganic Reactions					
Subject	Theory of Organic Reactions					
Code	V11G201V01417					
Study programme	Grado en Química					
Descriptors	ECTS Credits	Choose Ye	ar	0	uadmest	er
	6	Optional 4th	1	 2r	nd	_
Teaching language	Spanish					
Department	· · · · · · · · · · · · · · · · · · ·					
Coordinator	Vaz Araújo, Belén					
Lecturers	Vaz Araújo, Belén					
E-mail	belenvaz@uvigo.es					
Web						
	behaviors. English Friendly Program: Foreign student bibliographical references in English for th assessment tests in English.	is may request from the teaching st ne follow-up of the subject; b) attend	aff: a) mate d tutorials in	rial an Engli	id sh; c)	
Training an	d Learning Results					
Code						
A4 Student	s can communicate information, ideas, pro	blems and solutions to both special	ist and non-	specia	list audi	ences
A5 Student high de	s have developed those learning skills that gree of autonomy	are necessary for them to continue	e to undertal	ke furt	her stud	y with a
B5 Ability t	o adapt to new situations and to make dec	isions				
C44 Know th	e main methods for the study of organic re	eactions mechanisms				
D2 Capacit	y for teamwork					
D3 Ability t	o communicate in both oral and written for	m in Spanish and / or Galician and /	or English			
Expected re	esults from this subject					
Expected res	ults from this subject		Т	raining	g and Lea Results	arning
Understandi characteristi	ng the principles and theories related to the cs.	e main types of chemical reactions a	and theirA4 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 int	ermediates.	A4	B5	C44	D3

A5Rigorously apply the corresponding safety and healthy standards in the laboratory, as well as the
proper treatment of the waste generatedB5C44D2Collect data and write in the laboratory notebook, in a clear, concise and rigorous way, the
experiments carried out and the conclusions drawn.A4B5D2D3

Contents	
Торіс	
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	

correlation. Practice 2. Study of the primary isotope effect

in the oxidation of 1-phenylethanol

Planning Class hours Hours outside the Total hours classroom 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.	20	A4 A5	C4	4 D3
	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.				
Laboratory practical	 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. In addition, it will be evaluated (20%): the laboratory notebook the resolution of the questions raised in relation to the practices carried out. In order for students to pass the subject, they must obtain the PASS 	20	A5	B5 C4	4 D2 D3
	mark in the laboratory practice work.				
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	20	A4 A5	B5 C4	4 D3
	weighted grade of the global evaluation test.				
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 C4	4 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 C4	4 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 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