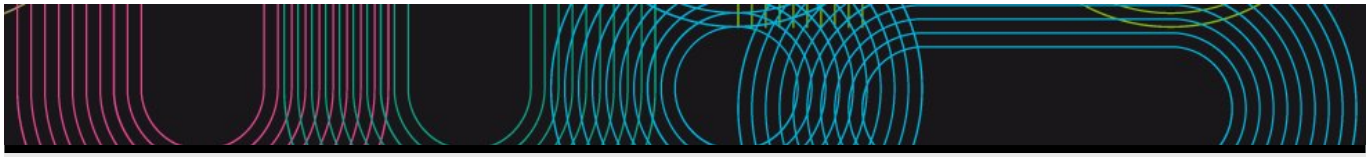

IDENTIFYING DATA				
Organic Chemistry III: Concerted, Radical and Photochemical Reactions				
Subject	Organic Chemistry III: Concerted, Radical and Photochemical Reactions			
Code	V11G201V01305			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	#EnglishFriendly Spanish Galician			
Department				
Coordinator	Nieto Faza, Olalla			
Lecturers	Gómez Bouzó, Uxía Gómez Pacios, María Generosa Nieto Faza, Olalla Silva López, Carlos			
E-mail	faza@uvigo.es			
Web				
General description	This class will study radical, pericyclic and photochemical processes, using a mechanistic approximation with emphasis on selectivity. The teaching methodology is centered around problem-solving, and includes laboratory and molecular modeling practical work. Subject in the English Friendly program: International students can ask the instructors for a) learning materials and bibliography in English, b) personal attention in English at office hours and c) assignments and exams in English.			

Training and Learning Results	
Code	
A3	Students have the ability to gather and interpret relevant data (usually within their field of study) to inform judgments that include reflection on relevant social, scientific or ethical issues
A4	Students can communicate information, ideas, problems and solutions to both specialist and non-specialist audiences
B3	Ability to manage information
B4	Ability for analysis and synthesis
C18	Know the properties of aliphatic, aromatic, heterocyclic and organometallic compounds
C19	Know the main synthesic routes in organic chemistry, including the interconversions of functional groups and the formation of carbon-carbon and carbon-heteroatom bonds
C27	Demonstrate the ability to observe, monitor and measure chemical processes, by systematically and reliably recording them and presenting reports of the work done
C28	Interpret data derived from laboratory observations and measurements in terms of their meaning and relate them to the appropriate theory
D3	Ability to communicate in both oral and written form in Spanish and / or Galician and / or English

Expected results from this subject	Training and Learning Results			
Know and apply the factors affecting the stability of organic radicals.	A3 A4	B3 B4	C18 C19	D3
Identify and understand the mechanisms of radical reactions and use this knowledge to propose strategies to either avoid or exploit them.	A3 A4	B3 B4	C18 C19	D3

Use the Woodward-Hoffmann rules to differentiate between allowed and forbidden reaction paths in pericyclic processes.	A3 A4	B3 B4	C18 C19	D3
Recognize the most common pericyclic mechanisms (electrocyclizations, cycloadditions, and sigmatropic and ene reactions) and use them in synthetic sequences.	A3 A4	B3 B4	C18 C19	D3
Predict the regio and stereoselectivity of pericyclic reactions.	A3 A4	B3 B4	C18 C19	D3
Understand the mechanisms of photochemical activation of organic molecules.	A3 A4	B3 B4	C18 C19	D3
Understand and apply the mechanisms of photochemical reactions: double bond isomerizations, photodissociations, photoreductions and pericyclic reactions.	A3 A4	B3 B4	C18 C19	D3
Perform pericyclic, radical and photochemical reactions and elaborate, separate and purify their products using common techniques.	A3 A4	B3 B4	C18 C19 C27 C28	D3
Use spectroscopic tools to establish the structure of organic compounds.	A3 A4	B3 B4	C18 C27 C28	D3
Use molecular modeling tools to study the properties of organic compounds and reaction mechanisms.	A3 A4	B3 B4	C18 C19 C27 C28	D3

Contents

Topic	
1. Reaction mechanisms	1.1. Reaction mechanism. Reaction profiles and transition state theory. 1.2. Reaction driving force. Frontier orbital theory. 1.3. Types of selectivity in organic transformations. 1.4. Mechanism classifications.
2. Radical reactions	2.1. Homolytic vs. heterolytic bond breaking. 2.2. Radical stability. 2.3. Chain reactions, alkane halogenation. 2.4. Radical polymerizations. 2.5. Radical reductions and reductive couplings. 2.6. Radical reactions in nature.
3. Pericyclic reactions	3.1. Woodward-Hoffmann rules. Orbital symmetry conservation and transition state aromaticity. Thermal and photochemical allowed and forbidden reactions. 3.2. Electrocyclizations. 3.3. Cycloadditions. Frontier orbital theory. 3.4. Sigmatropic and ene reactions.
4. Photochemical reactions	4.1. UV/vis spectra of organic molecules. Properties of excited states. 4.2. Photophysical processes: unimolecular deactivation, internal conversion, intersystem crossing, emission (fluorescence, phosphorescence). 4.3. Double bond isomerizations. 4.4. Photodissociations. 4.5. Photoreductions. 4.6. Pericyclic reactions. 4.7. Photochemical reactions in nature.
5. Laboratory work	Practical work on experiments related to the previous sections of the course. Synthesis, purification and characterization of organic compounds.
6. Molecular modeling	Use of computational chemistry tools to study the properties of organic molecules and reaction mechanisms associated to the previous sections of the course.

Planning

	Class hours	Hours outside the classroom	Total hours
Introductory activities	0	2	2
Flipped Learning	12	20	32
Problem solving	24	44	68
Laboratory practical	28	10	38
Mentored work	0	8	8
Problem and/or exercise solving	2	0	2

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

Methodologies	
	Description
Introductory activities	Presentation of the course and instructors. Review of the syllabus and the structure of the course in the remote learning platform.
Flipped Learning	The interaction of the students with the materials available in the remote learning platform is expected, as is working on the activities proposed to prepare for class. Classroom time will be used to consolidate, review, clarify and apply the studied concepts.
Problem solving	Practical exercises and problems will be solved to apply the concepts developed in the flipped classroom sessions.
Laboratory practical	The students will perform in the laboratory basic techniques related to the synthesis, separation, purification and structural characterization of organic compounds. The work includes evaluation of risk, experiment planning and analysis of results. Molecular modeling techniques will be used to study the properties of organic compounds and selected reaction mechanisms. To be allowed in the laboratory, the student is required to perform a set of preliminary preparation tasks on the remote learning platform. The work will be carried out individually in 3.5 h sessions, and will be documented in a laboratory notebook. After the practical sessions, a paper will be prepared according to the instructions of the professors.
Mentored work	

Personalized assistance	
Methodologies	**Description**
Flipped Learning	Continuous evaluation provides both instructors and students with feedback about the evolution of student learning and students' strengths and weaknesses. Although instructors can set tutorial appointments for students they deem at risk, it is expected that the students will take responsibility for they own learning and ask for help when needed. Students can request personalized support from the instructors at any time along the course, in order to solve any problem related to the subject, to review difficult concepts or to ask for help with the assignments. Tutorial sessions can be held through office hours in person or online, using the virtual campus. Personalized attention will also be provided through e-mail or the forums in the remote learning platform.
Problem solving	Problem-solving sessions in small groups facilitates personalized support to the student as soon as difficulties arise. As in the previous section, personalized attention will be provided in office hours, as well as through e-mail or forums in the remote learning platform.
Laboratory practical	In the laboratory sessions, most individual problems will be solved in class. As in the previous section, personalized attention will be provided in office hours, as well as through e-mail or forums in the remote learning platform.
Mentored work	

Assessment			
	Description	Qualification	Training and Learning Results
Flipped Learning	Students must participate in class activities and interact with the contents planned in the online learning platform. The results of the tests and other online activities integrated in every lesson in the platform will be evaluated.	10	A3 B3 C18 D3 A4 B4 C19
Problem solving	Students must solve short questions, problems and exercises, actively participating in the seminar sessions and completing them with independent work. A series of assignments will be graded. The grading will take into account the correctness of the provided answers, the quality of argumentation and the presentation of the results.	15	A3 B3 C18 D3 A4 B4 C19
Laboratory practical	The competencies associated to the safe handling of chemicals, the assessment of risks in the laboratory and the planning and execution of experiments (both computational and in the laboratory) and the analysis of results, will be evaluated. For this, we will use the systematic observation of the student's work, the preliminary work, previous to the laboratory sessions, and the quality of the laboratory notebook and the assigned report. The laboratory work will get a PASS/FAIL grade. Attendance to laboratory sessions and a PASS grade in them is needed to pass this course. 10% of the final grade is associated to an assignment related to the practical sessions.	10	

Mentored work	The students will work on the elaboration of documents in different formats, associated to the contents of the course.	10	
Problem and/or exercise solving	There will be three exams, involving problems and exercises: 1. A test about the first sections of the subject (2 hours), associated to a 15% of the final grade. 2. A test about all the contents covered in the class (2 hours), associated to a 40% of the final grade. A minimum grade of 4.0 out of 10 is required for a global passing grade. 3. A written exam (0.5 hours) related to the experimental part of the subject, associated to a 10% of the final grade. A 4.0 grade (out of 10) in this test is required for a global passing grade.	55	A3 B3 C18 D3 A4 B4 C19 C27 C28

Other comments on the Evaluation

Students need to demonstrate complete mastery of a set of essential learning outcomes in order to pass the course.

In case there is doubt about the mastery of the course's learning outcomes by any student, further or complementary oral tests can be scheduled for a sound evaluation.

Student participation in any of the graded activities will result in the assignment of a grade in this course (the student will be considered "presentado"). Attendance to laboratory sessions, participation in exams and the handing out of assignments are considered graded activities in this context.

Students who have attended the course in previous academic years: Those evaluated with a PASS grade in the experimental part of the course, upon request, will be awarded a PASS grade in this part of the course this year. As a result, their attendance to the laboratory sessions will not be required. However, assignments and the written test associated to the experimental part are required to achieve the grades associated to the experimental contents of the course this year (20%).

In the 2ª Edición de la Convocatoria Ordinaria, the grades obtained by the student in the problem solving, flipped learning and laboratory practical parts will be kept. An exam covering all the theoretical contents of the subject will be proposed, with a qualification that will represent a 45% of the final grade. A written test covering the experimental work will also be administered, with a contribution of 10% to the final grade. A minimum grade of 4.0 out of 10 in each of these two tests is needed for a passing grade and the consideration of the other grading elements.

The students desiring to opt-out of the continuous evaluation mode, need to attend the laboratory sessions and obtain a PASS in them, as well as obtaining a grade equal or higher than 5 out of 10 in the written test associated to the experimental part of the class (20% of the grade). On top of that, a grade equal or higher to 5 out of 10 is needed in a written exam covering all the contents of the course (80% of the grade).

Sources of information

Basic Bibliography

Eric V. Anslyn, Dennis A. Dougherty, **Modern physical organic chemistry**, University Science Books, 2006

Felix A. Carroll, **Perspectives on structure and mechanism in organic chemistry**, John Wiley, 2010

John Perkins, **Radical chemistry : the fundamentals**, Oxford University Press, 2000

Ian Fleming, **Pericyclic reactions**, Oxford University Press, 1999

Carol E. Wayne, Richard P. Wayne, **Photochemistry**, Oxford University Press, 1996

Steven M. Bachrach, **Computational organic chemistry**, John Wiley & Sons,, 2007

James W. Zubrick, **The Organic Chem Lab Survival Manual: a student's guide to techniques**, John Wiley & Sons, 2009

Jerry R. Mohrig ... [et al.], **Laboratory techniques in organic chemistry : supporting inquiry-driven experiments**, W.H. Freeman, 2014

Complementary Bibliography

Nicholas J. Turro, V. Ramamurthy, J.C. Scaiano, **Modern molecular photochemistry of organic molecules**, University Science Books, 2010

Ernö Pretsch, Philippe Buhlmann, Martin Badertscher, **Structure determination of organic compounds : tables of spectral data**, Springer,, 2009

Chemistry Libre Texts, **ChemistryLibre Texts**, ookshelves/Organic_Chemistry,

James Ashenhurst, **MasterOrganicChemistry**, https://www.masterorganicchemistry.com/,

Recommendations

Subjects that continue the syllabus

Organic Chemistry IV: Design of Organic Synthesis/V11G201V01310

Subjects that are recommended to be taken simultaneously

Physical Chemistry III: Quantum Chemistry/V11G201V01303

Subjects that it is recommended to have taken before

Structural Determination/V11G201V01206
Organic chemistry I/V11G201V01205
Organic chemistry II/V11G201V01210

Other comments

In this class, the student is expected to learn how to deftly manipulate a relevant number of new concepts in a short period of time. As a result, daily work and study is a must. The same applies to class attendance and active participation in all the proposed activities, including interaction with the materials available in the online platform or the reading of the designated documents before every in person session.

It is strongly advised to have passed Organic Chemistry I and II and Structural Determination or equivalent, since the concepts learnt in these classes will be required in this one.

The use of molecular models is heavily recommended, as one of the main difficulties of this course is the visualization of the three-dimensional structure of molecules.

A laboratory coat and notebook is needed for the laboratory sessions.