Teaching Guide				
Identifying Data				2020/21
Subject (*)	Elucidation of Reaction Mechanisms		Code	610500013
Study programme	Mestrado Universitario en Ciencias, Tecnoloxías e Xestión Ambiental (plan 2012)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	2nd four-month period	First	Optional	3
Language	SpanishGalicianEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Canle López, Moisés	E-mail	moises.canle@udc.es	
Lecturers	Canle López, Moisés	E-mail	moises.canle@udc.es	
Web				
General description	The contents of the subject "Elucidation of Reaction Mechanisms" are oriented to complement previous knowledge from the graduation studies. Usually, reaction mechanisms are proposed for chemical processes without any indication of the experimental evidences that lead to such mechanism instead of any other. This subject will show which are such evidences and how they can be obtained. It is not frequent to face the planification of a research into how chemical reactions take places. This subject will face this kind of problem from a practical point of view. There are a number of techniques, direct and indirect evidences that allow the elucidation of the mechanism of a chemical process. Chemical reactivity is central to changes in nature, and the recognition of the different reaction mechanisms is fundamental to control chemicall process, from the kinetic, thermodyanic points of view or even from the point of view of the generated products.			
Contingency plan	1. Modifications to the contents Only in the case of a contingency that impedes face-to-face teaching, contents would be kept, but taught remotely by videoconference. In such case, practical lessons would be replaced by case-studies. 2. Methodologies *Teaching methodologies that are maintained All. Only in the case of a contingency that impedes face-to-face teaching, assessment would be made remotely. *Teaching methodologies that are modified 3. Mechanisms for personalized attention to students On-demand tutorials with the lecturer (previously scheduled by e-mail) 4. Modifications in the evaluation Only in the case of contingency that impedes face-to-face teaching, assessment would be made remotely. *Evaluation observations: 5. Modifications to the bibliography or webgraphy Not necessary.			

Study programme competences / results	
Code	Study programme competences / results
A1	Coñecemento das realidades interdisciplinares da Química e do Medio Ambiente, dos temas punteiros nestas disciplinas e das perspectivas de futuro.
A3	Capacitar ao alumno para o desenvolvemento dun traballo de investigación nun campo da Química ou do Medio Ambiente, incluíndo os procesos de caracterización de materiais, o estudo das súas propiedades fisicoquímicas e biolóxicas e dos procesos que poden sufrir no medio natural.

A4	Coñecer en profundidade as características e fundamentos de diversos modelos químicos para o estudo de sistemas orgánicos, inorgánicos e biolóxicos, incluídos os materiais con proxección tecnológica.
A6	Coñecemento do comportamento de diferentes especies químicas e dos procesos aos que poden estar sometidas unha vez liberadas no medio ambiente, incluíndo as súas relacións entre distintos compartimentos ambientais.
A7	Coñecer o marco teórico e as aplicacións da electroquímica e da fotocatálise nos campos da enerxía e o medio ambiente.
A8	Coñecer os fundamentos das interaccións intermoleculares e as súas aplicacións no campo da catálise supramolecular,recoñecemento molecular e biocatálise.
A9	Coñecer algunhas aplicacións básicas da química computacional e dos programas de cálculo máis utilizados nos ámbitos da química e o medio ambiente.
A11	Coñecer as distintas técnicas experimentais e computacionales orientadas á caracterización de mecanismos de reacción.
A20	Coñecemento dos principais tipos de produtos naturais: enzimas, receptores moleculares, etc. Entender a súa participación en procesos de catálise e autoensamblaxe.
A22	Dominar as técnicas instrumentais de análises máis típicas no ámbito químico profesional.
B1	Posuír e comprender coñecementos que acheguen unha base ou oportunidade de ser orixinais no desenvolvemento e/ou aplicación de ideas, a miúdo nun contexto de investigación.
B2	Que os estudantes saiban aplicar os coñecementos adquiridos e a súa capacidade de resolución de problemas en contornas novas ou pouco coñecidos dentro de contextos máis amplos (ou multidisciplinares) relacionados coa súa área de estudo.
B3	Que os estudantes sexan capaces de integrar coñecementos e enfrontarse á complexidade de formular xuízos a partir dunha información que, sendo incompleta ou limitada, inclúa reflexións sobre as responsabilidades sociais e éticas vinculadas á aplicación dos seus coñecementos e suizos.
B4	Que os estudantes saiban comunicar as súas conclusións e os coñecementos e razóns últimas que as sustentan a públicos especializados e non especializados dun modo claro e sen ambigüedades.
B5	Que os estudantes posúan as habilidades de aprendizaxe que lles permitan continuar estudando dun modo que haberá de ser en gran medida autodirixido ou autónomo.
B6	Ser capaz de analizar datos e situacións, xestionar a información dispoñible e sintetizala, todo iso a un nivel especializado.
B7	Ser capaz de planificar adecuadamente desenvolvementos experimentais, a un nivel especializado.
C1	Ser capaz de traballar en equipos, especialmente nos interdisciplinares e internacionais.
C2	Ser capaz de manter un pensamento crítico dentro dun compromiso ético e no marco da cultura da calidade.
C3	Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado.
C4	Expresarse correctamente, tanto de forma oral coma escrita, nas linguas oficiais da comunidade autónoma.
C5	Dominar a expresión e a comprensión de forma oral e escrita dun idioma estranxeiro.
C9	Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben enfrontarse.
C10	Asumir como profesional e cidadán a importancia da aprendizaxe ao longo da vida.
C11	Valorar a importancia que ten a investigación, a innovación e o desenvolvemento tecnolóxico no avance socioeconómico e cultural da sociedade.

Learning outcomes			
Learning outcomes	Study programme competences / results		
To go deeper into the physical basis of chemical reactivity.	AC4 AC6 AC7 AC8 AC9 AC20	BC1 BC2	CC1 CC3 CC9 CC11
To expand the knowledge and ability to use experimental techniques to determine and measure chemical reactivity and its changes.	AC11 AC22	BC7	

To understand the different concepts and theories necessary to characterize chemical processes and their course.	AC4 AC7 AC9	BC2 BC3 BC6	CC1 CC3 CC9 CC11
To be able to use different instruments that are frequently used for the charecterization of reaction mechanisms.	AC9 AC11 AC22	BC3 BC7	CC3
To be able to use / apply acquired abilities and concepts for the resolution of practical exemples..	AC1 AC3 AC4 AC6	BC2 BC3 BC4 BC5 BC6	CC2 CC3 CC4 CC5 CC9 CC10 CC11

Contents	
Topic	**Sub-topic**
Reaction media	Variables that influence chemical processes. Role of reaction medium in chemical processses
Reaction mechanisms	Classification of reaction mechanisms Kinetic and thermodynamic characteristics of the main reaction mechanisms
Experimental techniques for the elucidation of reaction mechanisms	Batch methods Continuous methods Techniques for the study of rapid and ultrarapid reactions
Chemical reactivity	Catalysis Kinetic isotope effects Linear free energy relationships (LFER) and queantitative structure-activity relationships
Photochemistry and photocatalysis	General concepts Photochemical processes Photochemistry, photocatalysis and photoreactivity

Planning				
Methodologies / tests	**Competencies / Results**	**Teaching hours (in-person & virtual)**	**Student?s personal work hours**	**Total hours**
Guest lecture / keynote speech	A1 A4 A6 A7 A8 A9 A11 A20 A22 B1 B5 C10	14	28	42
Case study	A3 B2 B3 B4 B6 B7 C2 C3 C4 C5 C9 C11	5	7.5	12.5
Laboratory practice	B2 B4 B6 C1 C4 C5	8	10	18
Objective test	A4 A6 A7 A8 A9 A11 A20 A22 B2 B3 B4 B6	1.5	0	1.5
Personalized attention		1	0	1
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	**Description**

Guest lecture / keynote speech	? Two-hour sessions to present the masterlines of the subject, indicationg the students the most relevant points to take into account when studying and recommeding appropriate materials for a better comprehension. ? The students will have the audiovisual material available through the Moodle virtual plattform.
Case study	? Different real cases will be critically analyzed and discussed, in order to apply the acquired knowledge
Laboratory practice	? Will take place in the laboratory, in the days and hours that will be announces. ? At the end of the practical lessons, the student will hand a report on the experimental project developed, and realize a short oral presentation analyzing the experimental part and the meaning of the obtained results.
Objective test	? There will be a short exam, that may include both theory and practice

Personalized attention	
Methodologies	**Description**
Case study Laboratory practice	Will be carried out at the lecturers' offices, or at the Laboratory of Physical Chemistry I, according to the established timetable (consult for each lecturer). Proposed exercises, laboratory reports, etc. may be hand directly in these hours, solving any doubt or question about them. Doubt or questions with a simple and brief answer may be asked and answered through the Moodle virtual plattform. More complicated topics will need an appointment.

Assessment			
Methodologies	**Competencies / Results**	**Description**	**Qualification**
Case study	A3 B2 B3 B4 B6 B7 C2 C3 C4 C5 C9 C11	Evaluation will be centered in the critical analysis of the proposed cases, as well as on the suggestion of alternative solutions.	20
Objective test	A4 A6 A7 A8 A9 A11 A20 A22 B2 B3 B4 B6	May include short test or multiple choice questions or short problems / cases to analyze.	40
Laboratory practice	B2 B4 B6 C1 C4 C5	Both the experimental design and the critical analysis of the obtaind results will be evaluated.	40
Others			

Assessment comments
Para superar la asignatura habrá que asistir tanto a las prácticas de laboratorio como a las simulaciones, caso de haberlas.

Sources of information	
Basic	- H. Maskill (1985). The Physical Basis of Organic Reactivity. Oxford University Press Study materials or reference to them will be accesible through the Moodle virtual plattform.Study materials or reference to them will be accesible through the Moodle virtual plattform.
Complementary	- H. Maskill (Ed.), (2006). Investigating Organic Reaction Mechanisms . Blackwell Science - N. J. Turro; V. Ramamurthy; J.C. Scaiano (2009). Principles of Molecular Photochemistry. An Introduction. University Science Books - E.V. Anslyn, D.A. Dougherty (2006). Modern Physical Organic Chemistry. University Science Books

Recommendations
Subjects that it is recommended to have taken before
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus

Other comments
A higher profit from this subject would require actualized knowledge of Physical Chemistry. It is strongly recommeded to review the theoretical concepts introduced in the lessons through the resolution of questions, exercises and / or cases, that will be proposed.

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.