UNIVERSIDADE DA CORUÑA

Guía Docente				
Datos Identificativos				2016/17
Asignatura (*)	Elucidación de Mecanismos de Reacción		Código	610500013
Titulación				
Descriptores				
Ciclo	Período	Curso	Tipo	Créditos
Mestrado Oficial	2º cuadrimestre	Primeiro	Optativa	3
Idioma	CastelánGalegoInglés			
Modalidade docente	Presencial			
Prerrequisitos				
Departamento	Química Física e Enxeñaría Química 1			
Coordinación	Canle López, Moisés	Correo electrónico	moises.canle@udc.es	
Profesorado	Canle López, Moisés Fernandez Perez, Maria Isabel	Correo electrónico	moises.canle@udc.es isabel.fernandez.perez@udc.es	
Web				
Descrición xeral	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.			

Competencias / Resultados do título	
Código	Competencias / Resultados do título

Resultados da aprendizaxe			
Resultados de aprendizaxe	Competencias / Resultados do título		
To go deeper into the physical basis of chemical reactivity.	AM4 AM6 AM7 AM8 AM9 AM20	BM1 BM2	CM1 CM3 CM9 CM11
To expand the knowledge and ability to use experimental techniques to determine and measure chemical reactivity and its changes.	AM11 AM22	BM7	
To understand the different concepts and theories necessary to characterize chemical processes and their course.	AM4 AM7 AM9	BM2 BM3 BM6	CM1 CM3 CM9 CM11
To be able to use different instruments that are frequently used for the charecterization of reaction mechanisms.	AM9 AM11 AM22	BM3 BM7	CM3

To be able to use / apply acquired abilities and concepts for the resolution of practical exemples..	AM1 AM3 AM4 AM6	BM2 BM3 BM4 BM5 BM6	CM2 CM3 CM4 CM5 CM9 CM10 CM11

Contidos	
Temas	**Subtemas**
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	General concepts Photochemical processes Photochemistry and photoreactivity

Planificación				
Metodoloxías / probas	**Competencias / Resultados**	**Horas lectivas (presenciais e virtuais)**	**Horas traballo autónomo**	**Horas totais**
Sesión maxistral	A1 A4 A6 A7 A8 A9 A11 A20 A22 B1 B5 C10	10	20	30
Estudo de casos	A3 B2 B3 B4 B6 B7 C2 C3 C4 C5 C9 C11	4	6	10
Prácticas de laboratorio	B2 B4 B6 C1 C4 C5	15	18.75	33.75
Proba obxectiva	A4 A6 A7 A8 A9 A11 A20 A22 B2 B3 B4 B6	1	0	1
Atención personalizada		1	0	1
***Os datos que aparecen na táboa de planificación son de carácter orientativo, considerando a heteroxeneidade do alumnado**				

Metodoloxías	
Metodoloxías	**Descrición**
Sesión maxistral	? 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.
Estudo de casos	? Different real cases will be critically analyzed and discussed, in order to apply the acquired knowledge
Prácticas de laboratorio	? 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.

Proba obxectiva	? There will be a short exam, that may include both theory and practice

Atención personalizada	
Metodoloxías	**Descrición**
Estudo de casos Prácticas de laboratorio	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.

Avaliación			
Metodoloxías	**Competencias / Resultados**	**Descrición**	**Cualificación**
Estudo de casos	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
Proba obxectiva	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
Prácticas de laboratorio	B2 B4 B6 C1 C4 C5	Both the experimental design and the critical analysis of the obtaind results will be evaluated.	40
Outros			

Observacións avaliación
Para superar la asignatura habrá que asistir tanto a las prácticas de laboratorio como a las simulaciones.

Fontes de información	
Bibliografía básica	- 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.
Bibliografía complementaria	- 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

Recomendacións
Materias que se recomenda ter cursado previamente
Materias que se recomenda cursar simultaneamente
Materias que continúan o temario
Observacións
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 and exercises, that will be proposed.