



Guía Docente				
Datos Identificativos			2012/13	
Asignatura (*)	Elucidación de Mecanismos de Reacción	Código	610500013	
Titulación				
Descriptorios				
Ciclo	Período	Curso	Tipo	Créditos
Mestrado Oficial	2º cuatrimestre	Primeiro	Optativa	3
Idioma	CastelánGalegoInglés			
Prerrequisitos				
Departamento	Química Física e Enxeñaría Química 1			
Coordinación	Canle López, Moisés	Correo electrónico	moises.canle@udc.es	
Profesorado	Canle López, Moisés	Correo electrónico	moises.canle@udc.es	
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Web				
Descrición xeral	<p>The contents of the subject &quot;Elucidation of Reaction Mechanisms&quot; 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.</p> <p>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.</p> <p>Chemical reactivity is central to changes in nature, and the recognition of the different reaction mechanisms is fundamental to control chemical process, from the kinetic, thermodynamic points of view or even from the point of view of the generated products.</p>			

Competencias da titulación	
Código	Competencias da titulación

Resultados da aprendizaxe			
Competencias de materia (Resultados de aprendizaxe)	Competencias da titulación		
To go deeper into the physical basis of chemical reactivity.	AM4 AM6 AM7 AM8 AM20	BM1 BM2	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	BM2 BM3 BM6	CM3 CM9 CM11
To be able to use different instruments that are frequently used for the charecterization of reaction mechanisms.	AM11 AM22	BM3 BM7	CM3
To be able to use / apply acquired abilities and concepts for the resolution of practical exmples..	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 processes
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 quantitative structure-activity relationships
Photochemistry	General concepts Photochemical processes Photochemistry and photoreactivity

Planificación			
Metodoloxías / probas	Horas presenciais	Horas non presenciais / traballo autónomo	Horas totais
Sesión maxistral	10	20	30
Prácticas de laboratorio	15	18.75	33.75
Proba obxectiva	1	0	1
Estudo de casos	4	6	10
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, indicating the students the most relevant points to take into account when studying and recommending appropriate materials for a better comprehension. ? The students will have the audiovisual material available through the Moodle virtual platform.
Prácticas de laboratorio	? Will take place in the laboratory, in the days and hours that will be announced. ? 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
Estudo de casos	? Different real cases will be critically analyzed and discussed, in order to apply the acquired knowledge

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 platform. More complicated topics will need an appointment.

Avaliación



Metodoloxías	Descrición	Cualificación
Estudo de casos	Evaluation will be centered in the critical analysis of the proposed cases, as well as on the suggestion of alternative solutions.	20
Proba obxectiva	May include short test or multiple choice questions or short problems / cases to analyze.	40
Prácticas de laboratorio	Both the experimental design and the critical analysis of the obtained 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
Bibliografía complementaria	- H. Maskill (Ed.), (2006). Investigating Organic Reaction Mechanisms . Blackwell Science - E.V. Anslyn, D.A. Dougherty (2006). Modern Physical Organic Chemistry. University Science Books - N. J. Turro; V. Ramamurthy; J.C. Scaiano (2009). Principles of Molecular Photochemistry. An Introduction. 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 recommended to review the theoretical concepts introduced in the lessons through the resolution of questions and exercises, that will be proposed.

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