



Guía Docente

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Datos Identificativos				2022/23
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			
Coordinación	Canle López, Moisés	Correo electrónico	moises.canle@udc.es	
Profesorado	Canle López, Moisés	Correo electrónico	moises.canle@udc.es	
Web				
Descrición xeral	Os contidos da materia "Elucidación de Mecanismos de Reacción" orientanse a complementar coñecementos previos dos estudos de Grao. Polo xeral, os mecanismos de reacción se propoñen para os procesos químicos sn indicación das evidencias experimentais que conducen a dito mecanismo en lugar de outros posibles, e cómo se obteñen ditas evidencias. Non é habitual enfrontar a planificación dunha investigación sobre cómo teñen lugar os mecanismos de reacción. Esta materia aborda este problema dende un punto de vista práctico. Hai unha variedade de técnicas, evidencias directas e indirectas que permiten elucidar o mecanismo de reacción dun proceso químico. A reactividade química é central para os procesos de cambio na natureza, e coñecer os distintos mecanismos de reacción é fundamental para controlar os procesos químicos, tanto do punto de vista cinético como do termodinámico ou dos produtos de reacción xerados.			

Competencias / Resultados do título

Código	Competencias / Resultados do título
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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 examples..	AM1	BM2	CM2
	AM3	BM3	CM3
	AM4	BM4	CM4
	AM6	BM5	CM5
		BM6	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 and photocatalysis	General concepts Photochemical processes Photochemistry, photocatalysis 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	16	32	48
Estudo de casos	A1 A3 B2 B4 B6 B7 C2 C3 C1 C4 C5 C9 C11	10	15	25
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, 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.
Estudo de casos	? 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



Atención personalizada

Metodoloxías	Descrición
Estudo de casos	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	Competencias / Resultados	Descrición	Cualificación
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.	50
Estudo de casos	A1 A3 B2 B4 B6 B7 C2 C3 C1 C4 C5 C9 C11	Both the experimental design and the critical analysis of the obtained results will be evaluated.	50
Outros			

Observacións avaliación

To pass the subject it will be necessary to attend at least 3/4 of the programmed sessions.

To pass the subject it will be necessary to pass at least 40% of both the "case-study" and the "objective test".

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 platform. Study materials or reference to them will be accesible through the Moodle virtual platform.
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 recommended to review the theoretical concepts introduced in the lessons through the resolution of questions, exercises and / or cases, that will be proposed.

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