Teaching Guide					
Identifying Data					2015/16
Subject (*)	Mecanismos de reacción e catálise			Code	610509009
Study programme	Mestrado en Investigación Química e Química Industrial				
Descriptors					
Cycle	Period	Year		Type	Credits
Official Master's Degree	1st four-month period	First		Optativa	3
Language	SpanishGalicianEnglish				
Teaching method	Face-to-face				
Prerequisites					
Department	Química Física e Enxeñaría Química 1				
Coordinador	Santaballa Lopez, Juan Arturo		E-mail	arturo.santaballa@udc.es	
Lecturers	Fernandez Perez, Maria Isabel Santaballa Lopez, Juan Arturo		E-mail	isabel.fernandez.perez@udc.es arturo.santaballa@udc.es	
Web	miiquimica.webnode.es/				
General description	A materia pertence á especialidade Estrutura e Reactividade Química, relaciónase fundamentalmente coas asignaturas da citada especialidade, así como con aquelas pertencentes o módulo de Formación Obrigatoria Avanzada. Igualmente relaciónase co Seminario de Master, Prácticas Académicas e Traballo de Fin de Master. Esta asignatura é esencial na especialidade Estrutura e Reactividade Química, aborda os aspectos esenciais para comprende-la reactividade química no seu aspecto máis amplo. Na comprensión da reactividade química é fundamental dispor dos coñecementos asociados á elucidación dos mecanismos de reacción. Os contidos docentes desta materia supoñen, por unha parte, unha profundización en diversos aspectos dos tratados no módulo de Formación Obrigatoria Avanzada e, por outra, o complemento necesario para as outras materias da especialidade: Modelización Molecular, Química Supramolecular e Espectroscopia de Fluorescencia e Fotoquímica.				

Study programme competences	
Code	Study programme competences

Learning outcomes			
Learning outcomes	Study programme competences		

Contents	
Topic	Sub-topic
Estructura química, reactividade e actividade	Definición de reactividade e actividade. Relación entre estrutura química, reactividade e actividade. Reactividade química e mecanismos de reacción.
Reactividade química en fase homoxénea e heteroxénea, incluindo sistemas macro, micro e nanoscópicos	Reactividade química en fase homoxénea. Reactividade química en fase heteroxénea. Reactividade química en sistemas macro, micro e nanoscópicos. Estudio de casos.
Métodos experimentais no estudo da reactividade química	Mecanismos de reacción e análise de produtos. Principais métodos experimentais. Intermedios e mecanismos de reacción Cinética química en sistemas multifásicos. Estudio de casos.
Modelos teóricos e/ou empíricos relacionados coa reactividade e os mecanismos de reacción incluindo relacións cuantitativas estrutura-actividade (QSAR)	Relacións lineais de enerxía libre. Teoría de Marcus. Relacións QSAR: indicadores de reactividade e de actividade. Estudio de casos.
Catalizadores para a protección ambiental e os catalizadores do futuro	Preparación e caracterización de catalizadores. Catálise e protección medioambiental. Os catalizadores do futuro. Estudio de casos.

Planning

Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Seminar		9	18	27
Case study		0	7	7
Workbook		0	3	3
Mixed objective/subjective test		2	0	2
Guest lecture / keynote speech		12	24	36
Personalized attention		0		0
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	Description
Seminar	
Case study	
Workbook	
Mixed objective/subjective test	
Guest lecture / keynote speech	

Personalized attention	
Methodologies	Description
Seminar	

Assessment			
Methodologies	Competencies	Description	**Qualification**
Seminar			20
Case study			15
Workbook			5
Mixed objective/subjective test			60

Assessment comments

Sources of information

Basic	Howard Maskill (editor): The Investigation of Organic Reactions and their Mechanisms, Blackwell Publishing, 2006 (ISBN-13: 978-1-4051-3142-1).Howard Maskill: The Physical Basis of Organic Chemistry Publisher, Oxford University Press,1986 (ISBN-13: 978-0198551997). Stephen R. Schmidt (editor): Catalysis of Organic Reactions, CRC Press (Taylor & Francis Group), 2007 (ISBN 0?8493?7557?6). John Regalbuto (editor): Catalyst Preparation. Science and Engineering. CRC Press (Taylor & Francis Group), 2007Â (ISBN-13: 978-0-8493-7088-5). Vasile I. Parvulescu & Christopher Hardacre: Catalysis in Ionic Liquids, Chem. Rev. 2007, 107, 2615-2665. Smiljko Asperger: Chemical Kinetics and Inorganic Reaction Mechanisms, Springer,Â 2012 (ISBN-13: 978-1461348719). Eric V. Anslyn & Dennis A. Dougherty: Modern Physical Organic Chemistry, University Science, 2005 (ISBN-13: 978-1891389313). Michael B. Sponsler: Student Solutions Manual To Accompany Modern Physical Organic Chemistry, Univ Science Books, 2005 (ISBN-13: 978-1891389368). D. K. Chakrabarty & B. Viswanathan: Heterogeneous Catalysis, New Age Science, 2009 (ISBN-13: 978-1906574093). Julian R.H. Ross: Heterogeneous Catalysis: Fundamentals and Applications, Elsevier, 2011 (ISBN-13: 978-0444533630). Steven L Suib: New and Future Developments in Catalysis: Hybrid Materials, Composites, and Organocatalysts, Elsevier, 2013 (ISBN-13: 978-0444538765). Monika Nendza: Structure - Activity Relationships in Environmental Sciences, Series: Chapman & Hall Ecotoxicology Series (Book 6), Springer, 2013 (ISBN-13: 978-1461376606). Kamel Mansouri: Estimating degradation and fate of organic pollutants by QSAR modeling: Contributing to the implementation of REACH, the European Community regulation on chemicals, LAP LAMBERT Academic Publishing, 2013 (ISBN-13: 978-3659447662)Howard Maskill (editor): The Investigation of Organic Reactions and their Mechanisms, Blackwell Publishing, 2006 (ISBN-13: 978-1-4051-3142-1).Howard Maskill: The Physical Basis of Organic Chemistry Publisher, Oxford University Press,1986 (ISBN-13: 978-0198551997). Stephen R. Schmidt (editor): Catalysis of Organic Reactions, CRC Press (Taylor & Francis Group), 2007 (ISBN 0?8493?7557?6). John Regalbuto (editor): Catalyst Preparation. Science and Engineering. CRC Press (Taylor & Francis Group), 2007 (ISBN-13: 978-0-8493-7088-5). Vasile I. Parvulescu & Christopher Hardacre: Catalysis in Ionic Liquids, Chem. Rev. 2007, 107, 2615-2665. Smiljko Asperger: Chemical Kinetics and Inorganic Reaction Mechanisms, Springer, 2012 (ISBN-13: 978-1461348719). Eric V. Anslyn & Dennis A. Dougherty: Modern Physical Organic Chemistry, University Science, 2005 (ISBN-13: 978-1891389313). Michael B. Sponsler: Student Solutions Manual To Accompany Modern Physical Organic Chemistry, Univ Science Books, 2005 (ISBN-13: 978-1891389368). D. K. Chakrabarty & B. Viswanathan: Heterogeneous Catalysis, New Age Science, 2009 (ISBN-13: 978-1906574093). Julian R.H. Ross: Heterogeneous Catalysis: Fundamentals and Applications, Elsevier, 2011 (ISBN-13: 978-0444533630). Steven L Suib: New and Future Developments in Catalysis: Hybrid Materials, Composites, and Organocatalysts, Elsevier, 2013 (ISBN-13: 978-0444538765). Monika Nendza: Structure - Activity Relationships in Environmental Sciences, Series: Chapman & Hall Ecotoxicology Series (Book 6), Springer, 2013 (ISBN-13: 978-1461376606). Kamel Mansouri: Estimating degradation and fate of organic pollutants by QSAR modeling: Contributing to the implementation of REACH, the European Community regulation on chemicals, LAP LAMBERT Academic Publishing, 2013 (ISBN-13: 978-3659447662)
Complementary	

Recommendations
Subjects that it is recommended to have taken before
Profundización en Química Analítica/610509001
Profundización en Química Física/610509002
Profundización en Química Orgánica/610509004
Profundización en Química Inorgánica/610509003
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments

(*)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.