Teaching Guide				
Identifying Data				2018/19
Subject (*)	Organic Reactivity and Organometallic Chemistry		Code	610500020
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	Spanish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Ojea Cao, Vicente	E-mail	vicente.ojea@udc.es	
Lecturers	Ojea Cao, Vicente	E-mail	vicente.ojea@udc.es	
Web				
General description	This course focuses on the study of the structure, properties and reactivity of organic and organometallic compounds, both through experimental and computational techniques, with particular attention to synthetic applications of transition metals in organic synthesis.			

Study programme competences	
Code	Study programme competences
A1	Coñecemento das realidades interdisciplinares da Química e do Medio Ambiente, dos temas punteiros nestas disciplinas e das perspectivas de futuro.
A2	Deseño de novas especies químicas e materiais con propiedades determinadas.
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.
A5	Capacitación para o deseño de vías de síntese e retrosíntese de novos compostos.
A11	Coñecer as distintas técnicas experimentais e computacionales orientadas á caracterización de mecanismos de reacción.
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.
B6	Ser capaz de analizar datos e situacións, xestionar a información dispoñible e sintetizala, todo iso a un nivel especializado.
C3	Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado.
C5	Dominar a expresión e a comprensión de forma oral e escrita dun idioma estranxeiro.
C6	Utilizar as ferramentas básicas das tecnoloxías da información e as comunicacións (TIC) necesarias para o exercicio da súa profesión e para a aprendizaxe ao longo da súa vida.
C9	Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben enfrontarse.
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		
Know in depth the characteristics and foundations of various models for the study of the structure, properties and reactivity of organic and organometallic compounds. Know and apply the basic techniques of computational chemistry in the study of the structure, properties and reaction processes of organic and organometallic compounds	AC1 AC3 AC4 AC11	BC1 BC2 BC4 BC6	CC6 CC9
Qualification for designing retrosynthetic analysis and synthetic routes by using organometallic reagents	AC1 AC2 AC5	BC1 BC2 BC3 BC6	CC3 CC5 CC9 CC11

Contents	
Topic	Sub-topic
Chapter 1: Steric, conformational and stereoelectronic control of the reactivity	1.1 Enantiomers, diastereomers, prochirality. 1.2. Conformational analysis. 1.3 Computational methods for the conformacional analysis: molecular mechanics, electronic structure methods. 1.4 Stereoelectronic effects and reactivity. 1.5 Baldwin rule´s. Winstein-Holmes ecuation and Curtin-Hammett prionciple
Chapter 2: Organometallic Chemistry in Organic Synthesis	2.1 Organometallic chemistry in organic synthesis: fundamentals and reaction mechanisms; 2.2 Cross-coupling reactions; 2.3 Reactions of alkenes and alkynes: insertion, electrophilic addition and carbonylation; 2.4 Reactions of carbenes; 2.5 Reactions of C-H activation
Experiment 1	Resolution of problems related to the analysis of the reactivity of organic compounds by computational methods.
Experiment 2	Experimental work in one of the reactions previously studied

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A1 A2 A3 A4 A5 A11 C5	12	0	12
Laboratory practice	A2 A3 A5 A11 B1 B2 B6 C6	8	4	12
Supervised projects	A11 B1 B2 B6 C3 C6	0	23	23
Seminar	A3 A4 A5 B2 B3 B4 B6 C3 C5 C9 C11	2	22	24
Oral presentation	A3 A4 A11 B1 B2 B4 C11	1	2	3
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	Development of the fundamental contents of the program by means of theoretical explanations and practical examples.
Laboratory practice	Realization of an experimental procedure of organometallic chemistry. Analysis and resolution of selected problems by computational methods.
Supervised projects	Computational analysis of a reaction process and elaboration of a short presentation of the results obtained
Seminar	Exercises related with the contents of organometalic chemistry will be solved in the seminars. The students will have to prepare written solutions, deliver them to the professor and expose them during the seminar
Oral presentation	Oral presentation of the supervised project about molecular modelling

Personalized attention	
Methodologies	**Description**
Seminar Supervised projects Laboratory practice	The student will have the help of the professor for the resolution of the doubts that could pose him during the preparation of the projects

Assessment			
Methodologies	**Competencies**	**Description**	**Qualification**
Seminar	A3 A4 A5 B2 B3 B4 B6 C3 C5 C9 C11	The solutions written by the students and the oral presentations about the problems posed on organometalic chemistry will be evaluated	40
Supervised projects	A11 B1 B2 B6 C3 C6	Evaluation of the computational analysis performed by the student on a system of his interest	30
Laboratory practice	A2 A3 A5 A11 B1 B2 B6 C6	Continuous evaluation of the work in the laboratory will take into account the interest and the attitude of the student and the skills reached in the experimental procedures and the utilization of the computational tools for the molecular modellization of the reaction process	20
Oral presentation	A3 A4 A11 B1 B2 B4 C11	Assessment of the oral presentation about molecular modelling of reaction process	10

Assessment comments
All activities are mandatory

Sources of information	
Basic	- Robinson, M. J. T (). Organic Stereochemistry. Oxford: University Press - Eliel, E. L (). Stereochemistry of Organic Compounds. New York: Wiley - Foresman, J. B.; Frisch, A. (1996). Exploring Chemistry with Electronic Structure Methods. Pittsburg, PA: Gaussian - Hegedus, L. S. (). Transition Metals in the Synthesis of Complex Organic Molecules. Mill Valley: University Science Books - Bates, R. (). Organic Synthesis using Transition Metals Second edition . Blackwell
Complementary	

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

(*)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.