UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2021/22
Subject (*)	Synthetic Applications of Organometallic compounds		Code	610509112
Study programme	Mestrado Universitario en Investigación Química e Química Industrial (Plan 2020)			
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	Sarandeses Da Costa, Luis Alberto	E-mail	luis.sarandeses@udc.es	
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Web	www.usc.es/gl/centros/quimica/curso/master.html			
General description	This matter is basic in the specialty Synthetic Chemistry because it studies the reactivity of organometallic compounds and their applications in synthesis and catalysis. The concepts addressed in this matter are useful in others of other modules such as Chemical Structure and Reactivity, Nanochemistry and New Materials and Biological Chemistry. This matter is related to others such as Organometallic Compounds and Advanced Coordination Chemistry, which cover general aspects of the structure and reactivity of the organometallic compounds and the coordination metal complexes. The use of organometallic compounds and catalysis by transition metals are fundamental tools of today's synthetic chemistry, both in their academic and industrial aspects. The current organic synthesis involves the development of more selective and sustainable processes, objectives for which organometallic compounds and catalysis are frequently required.			

Contingency plan	1. Modifications to the contents - No changes will be made. 2. Methodologies *Teaching methodologies that are maintained - Guest lecture / keynote speech - Seminar - Mixed objective/subjective test *Teaching methodologies that are modified - All teaching methodologies will be carried out through Teams. 3. Mechanisms for personalized attention to students - Email: permanent. - Moodle: Daily; according to the needs of the students. - Teams: Master sessions, seminars, tutorials (2-6 h/week). 4. Modifications in the evaluation - Seminar: 60% The continuous evaluation will have a weight of 60% in the qualification of the subject and will consist of the following components: problem solving and practical cases, questions during the courses and attendance and participation. It goes from 40% to 60%. - Mixed objective/subjective test: 40% Mixed test that will be about the contents explained. Common to the rest of the universities participating in the master. It goes from 60% to 40%. *Evaluation observations: The mixed test will consist of a set of questions through Moodle or Forms to answer in a certain time. There are no minimum restrictions in the evaluated sections. If the students had difficulties in taking the mixed test, they would use phone calls or use an asynchronous evaluation method. Students with recognition of part-time dedication and academic exemption from attendance exemption: preparation of supervised works (60%) and mixed test (40%). 5. Modifications to the bibliography or webgraphy There are no modifications to the bibliography.

Study programme competences / results	
Code	Study programme competences / results
A1	Define concepts, principles, theories and specialized facts of different areas of chemistry.
A2	Suggest alternatives for solving complex chemical problems related to the different areas of chemistry.
A3	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
A6	Design processes involving the treatment or disposal of hazardous chemicals
A8	Analyze and use the data obtained independently in complex laboratory experiments and relating them with the chemical, physical or biological appropriate techniques, including the use of primary literature sources
B1	Possess knowledge and understanding to provide a basis or opportunity for originality in developing and / or applying ideas, often within a research context
B2	Students should apply their knowledge and ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.

B4	Students should be able to communicate their conclusions, and the knowledge and the reasons that support them to specialists and non-specialists in a clear and unambiguous manner
B5	Students must possess learning skills to allow them to continue studying in a way that will have to be largely self-directed or autonomous.
B7	Identify information from scientific literature by using appropriate channels and integrate such information to raise and contextualize a research topic
B10	Use of scientific terminology in English to explain the experimental results in the context of the chemical profession
B11	Apply correctly the new technologies to gather and organize the information to solve problems in the professional activity.

Learning outcomes			
Learning outcomes	Study programme competences / results		
To understand the basis of catalytic cycles from the point of view of reaction coordinates and potential energy surfaces.	AC1 AC6 AC8	BC5	
To understand the applications in synthesis of the diversity of processes of formation of bonds mediated by organometallic compounds.	AC2 AC3 AC6	BC1 BC2 BC4 BC7 BC10 BC11	
Propose synthetic sequences with key disconnections based on synthetic processes of organometallic compounds.	AC2 AC3 AC6	BC1 BC2 BC4 BC7 BC11	

Contents	
Topic	Sub-topic
Topic 1. Energy principles and fundamentals of organometallic catalytic cycles.	? General concepts ? Thermodynamics and kinetics of the catalytic cycle of reactions catalysed by transition metals. ? Application: Pd catalyzed cross coupling; Synergy between computational and experimental results.
Topic 2. Cross-coupling reactions and Heck reaction.	? Cross-coupling reactions. Generalities. Leaving groups. Metals. Selectivity. ? Carbon-carbon bond formation reactions: organometallic compounds of Li, Zn, Al, Zr, Sn, Cu; Compounds of B and Si; Other metals; Enolates. ? Carbon-heteroatom bond formation reactions. ? Heck reaction. Components of the reaction. Inter- and intramolecular reactions. Asymmetric Heck Reactions. Heck reactions with organometallic species.
Topic 3. Insertion reactions.	? Carbonylative reactions. Generalities. Mechanism. ? Carbonylative coupling reactions. ? Hydroformylation reactions. ? Carbonylation reactions with carbonyl complexes. ? Carboxylation. ? Decarbonylative reactions and decarbonylative couplings. ? Other insertion reactions with zirconium and titanium.

Topic 4. Reactions of n3-allyl complexes.	? Palladium n3-allyl complexes (1. Synthesis and properties; 2. Regioselectivity and stereoselectivity). ? Allylic substitution reactions catalyzed by palladium complexes (1. Allylic alkylation; 2. Amination, etherification and allyl reduction; 3. Cyclization reactions through alkene insertion processes; 4. Cycloaddition reactions via trimethylenemethane intermediates) . ? Allylic substitution reactions catalyzed by complexes of other transition metals (Iridium, Nickel, Iron, Molybdenum). ? Alkylation reactions with alkynes and alenes catalyzed by Rh complexes.
Topic 5. Reactions of electrophilic complexes of alkenes, alkynes, dienes and arenes.	? Alkyl insertion reactions and Heck, Suzuki, etc., tandem reactions. ? Insertion reactions mediated by other metals (Zr and Ti). ? Electrophilic additions on alkenes and alkynes. ? Reaction of Nicholas and Pauson-Khand. ? Reactions of alkenes with palladium in high oxidation state. ? Synthetic applications of n4-dienyl complexes and n6-arenes.
Topic 6. Reactivity of metal carbenes.	? Characteristics of carbenes. ? Carbenes of transition metals. Structure and types. ? Transformations involving carbenes of transition metals. ? Olefin metathesis.
Topic 7. Activation reactions of C-H bonds.	? Introduction to the activation of C-H bonds: relevancy, difficulties and mechanisms of activation. ? Reactions of insertion of carbenes and nitrenes ? Ir-catalyzed borilation reactions ? Functionalization of alkanes and arenes catalyzed by Pd(II): oxygenation, arylation, halogenation, oxidative Heck reaction.

Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Seminar	A1 A2 A3 A6 A8 B1 B2 B4 B5 B7 B10 B11	7	18	25
Mixed objective/subjective test	A1 A2 A3 B2 B5	3	0	3
Guest lecture / keynote speech	A1 A8 B1 B2 B7 B10 B11	12	33	45
Personalized attention		2	0	2
(*)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	Seminars held with teachers of the Master, or with professionals invited from industry, the administration or other universities. Interactive sessions related to the different subjects with debates and exchange of opinions with students. Resolution of practical exercises (problems, test questions, interpretation and processing of information, evaluation of scientific publications, etc.). Additionally, during the seminars the possibility of carrying out other methodologies is contemplated: - Works, individually or in groups, on scientific topics related to the different subjects of the Master. - Oral presentation of papers, reports, etc., including discussion with teachers and students. - Use of specialized computer programs and internet. Online teaching support (Virtual Campus).

Mixed objective/subjective test	A final written exam is scheduled, which will allow to objectively evaluate the degree of assimilation and the ability to apply the contents of the subject by the student. The objective test will include a unique type of questions, which will be related to the structure, reactivity and synthesis of organic compounds, and will allow to determine if the answers are correct.
Guest lecture / keynote speech	Theoretical classes. Lectures (use of blackboard, computer, cannon), complemented with the tools of virtual teaching.

Personalized attention	
Methodologies	**Description**
Seminar Guest lecture / keynote speech	Two individual or small group tutorials are programmed to check the comprehension of the subject and to complement the student's formation through solving doubts and other questions.

Assessment			
Methodologies	**Competencies / Results**	**Description**	**Qualification**
Seminar	A1 A2 A3 A6 A8 B1 B2 B4 B5 B7 B10 B11	Continuous evaluation will have a weight of 40% in the grade of the subject and will consist of the following components: problem solving and practical cases (15%), oral presentation [(practical cases, problems), 10%] and oral questions during Course (10%) and attendance and participation (10%).	40
Mixed objective/subjective test	A1 A2 A3 B2 B5	The final exam will cover all the contents of the subject.	60

Assessment comments
The evaluation of this subject will be done through continuous evaluation and the completion of a final exam. Repeating students will have the same attendance regime for classes as those who study the subject for the first time. Continuous evaluation (N1) will have a 40% weight in the subject's qualification and will consist of the following components: problem solving and practical cases (15%), oral presentation [(practical cases, problems), 10%] and questions Oral during the course (10%) and attendance and participation (10%). The final exam (N2) will cover all the contents of the subject. The qualification of the student will be obtained as a result of applying the following formula:Final note = maximum (0.4 x N1 + 0.6 x N2) N1 being the numeric note corresponding to the continuous evaluation (scale 0-10) and N2 the numerical note of the final exam (scale 0-10).

Sources of information	
Basic	- Bates, R. (2012). Organic Synthesis Using Transition Metals, 2nd Ed.. Wiley - Hegedus, L. S. (1999). Transition Metals in the Synthesis of Complex Organic Molecules, 2nd Ed.. University Science Books

Complementary	- Luther, G. W. (2016). Reactivity of Transition Metal Complexes: Thermodynamics, Kinetics and Catalysis, in Inorganic Chemistry for Geochemistry and Environmental Sciences: Fundamentals and Applications. Wiley - Cybulski, A.; Moulijn, J. A.; Stankiewicz, A. (2010). Novel Concepts in Catalysis and Chemical Reactors: Improving the Efficiency for the Future. Wiley-VCH - Ananikov, V. P. (2015). Understanding Organometallic Reaction Mechanisms and Catalysis: Computational and Experimental Tools. Wiley-VCH - Negishi, E., Ed. (2002). Handbook of Organopalladium Chemistry for Organic Synthesis. Wiley - De Meijere, A., Bräse, S., Oestreich, M. (2014). Metal-Catalyzed Cross-Coupling Reactions and More. Wiley-VCH - Beller, M., Bolm, C. (2004). Transition Metals for Organic Synthesis, 2nd Ed.. Wiley-VCH - Kazmaier, U. (2012). Transition Metal Catalyzed Enantioselective Allylic Substitution in Organic Synthesis. Springer-Verlag - Crabtree, R. H. (2005). The Organometallic Chemistry of the Transition Metals, 4th Ed.. Wiley - Yu, J.-Q. (2016). Science of Synthesis: Catalytic Transformations via C-H Activation Vol. 1 & 2. Thieme

Recommendations
Subjects that it is recommended to have taken before
Industrial Processes and Sustainability/610509104 Organometallic Chemistry/610509111 Advanced Structural Determination/610509103 Structure and Reactivity of Organic Compounds /610509114
Subjects that are recommended to be taken simultaneously
Stereoselective Synthesis/610509113
Subjects that continue the syllabus
Other comments