



| Teaching Guide | | | | |
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| Identifying Data | | | 2016/17 | |
| Subject (*) | Compostos organometálicos en síntese e catálise | Code | 610509011 | |
| Study programme | Mestrado en Investigación Química e Química Industrial (plan 2016) | | | |
| Descriptors | | | | |
| Cycle | Period | Year | Type | Credits |
| Official Master's Degree | Yearly | First | Optativa | 3 |
| Language | Spanish | | | |
| Teaching method | Face-to-face | | | |
| Prerequisites | | | | |
| Department | Química Fundamental | | | |
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| Lecturers | Sarandeses Da Costa, Luis Alberto | E-mail | luis.sarandeses@udc.es | |
| Web | | | | |
| General description | This subject, which belongs to Synthetic Chemistry block, studies the structure and reactivity of organometallic complexes and their catalytic applications in chemical synthesis. Also, this subject is essential for understanding other subjects of the Master belonging to the blocks of Biological Chemistry and Nanochemistry and New Materials. | | | |

| Study programme competences | |
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| Code | Study programme competences |
| 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 | Apply materials and biomolecules in innovative fields of industry and chemical engineering. |
| 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. |
| B3 | Students should be able to integrate knowledge and handle complexity, and formulate judgments based on information that was incomplete or limited, include reflecting on social and ethical responsibilities linked to the application of their knowledge and judgments. |
| 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 | | |
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| Learning outcomes | Study programme competences | |
| Predict the stability and reactivity of organometallic complexes according to their electronic characteristics.. | AC1 AC2 | BC1 BC2 BC3 BC7 BC10 BC11 |
| Propose reasonable mechanisms, based on the basic organometallic reactions, for reactions catalyzed for organometallic complexes. | AC1 AC2 AC3 | BC1 BC2 BC3 BC7 BC10 BC11 |



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| Use reasoning based on steric and electronic effects to predict how changes in reagents, metals and ligands affecting the course of reactions. | AC1 | BC1 BC2 BC3 |
| Propose synthetic routes with key steps based on organometallic complexes. | AC1 AC2 AC3 | BC1 BC2 BC3 |
| Read and critically interpret current scientific papers, with understanding and explanation of its contents and significance. | | BC1 BC7 BC10 BC11 |

| Contents | |
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| Topic | Sub-topic |
| Topic 1. General characteristics of organometallic complexes. | 1) Formalisms: a) oxidation state, b) electronic configuration, coordination number, and 18e- rule, c) classes of ligands. 2) Considerations about the bond. 3) Structural considerations. |
| Topic 2. Organometallic reactions mechanisms. | 1) Associative and dissociative mechanism. 2) Oxidative addition and reductive elimination. 3) Insertions and eliminations. 4) Attacks on nucleophilic and electrophilic ligands coordinated to the metal. 5) Transmetalation. |
| Topic 3. Cross-coupling reactions. Heck reaction. | 1) Cross-coupling reactions of Csp3 organometallic species. 2) Cross-coupling reactions of Csp2 organometallic species. 3) Cross-coupling reactions of Csp organometallic species. 4) Heck reaction. |
| Topic 4. Carbonylative and decarbonylative reactions. | 1) General Reactivity of metal carbonyls. 2) Carbonylative coupling reactions catalyzed by palladium and carbonylation of alkenes and alkynes. 3) Carbonylations of industrial interest: Monsanto process; hydroformylation (oxo process). 4) Decarbonylative reactions. |
| Topic 5. Metal-carbene complexes. | 1) Electrophilic carbenes (Fischer carbenes): preparation and reactivity. 2) Nucleophilic carbenes (Schrock carbenes). 3) Metathesis of alkenes: general mechanism, ROMP and RCM. |
| Topic 6. Metal-alkyne complexes. | 1) Structural Aspects. 2) Metal-alkyne stable complexes: complexes of Co as protecting groups of alkynes and Nicholas reaction. 3) Pauson-Khand reaction. 4) alkyne cycloaddition reactions. |
| Topic 7. Metal-alkene complexes, metal-diene and dienyl complexes. Reactions via η^3 -allyl complexes. Metal-arene complexes. | 1) Metal-alkene complexes of palladium and iron. 2) metal-diene: stabilization of allyl cations and nucleophilic addition. 3) Complexos η^5 -dienyl: synthetic applications. 6) Reactions of allylic substrates catalyzed by Pd, Ni and other metals. 7) Metal-arene complexes of groups 6 and 8 (Cr, Fe, Ru). |

| Planning | | | | |
|---------------------------------|---------------------------------|----------------------|-------------------------------|-------------|
| Methodologies / tests | Competencies | Ordinary class hours | Student?s personal work hours | Total hours |
| Problem solving | A1 A2 A3 B1 B2 B3 B7 B10 B11 | 9 | 0 | 9 |
| Mixed objective/subjective test | A2 A3 B2 B3 B11 | 2 | 0 | 2 |
| Guest lecture / keynote speech | A1 A2 A3 B1 B2 B3 B7 B10 B11 | 12 | 52 | 64 |
| 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 | |
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| Methodologies | Description |
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| Problem solving | Seminars with the Master's own teaching staff, guests or business professionals. Interactive sessions related to different subjects with discussions and exchange of views with students. Resolution of practical exercises (problems, multiple choice questions, interpretation and processing of information, evaluation of scientific publications, etc.). |
| Mixed objective/subjective test | The final exam will cover all the contents of the subject. |
| Guest lecture / keynote speech | Theoretical classes. Lectures (using slate, computer, projector), supplemented by their own online teaching tools. |

Personalized attention

| Methodologies | Description |
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| Problem solving | Os alumnos disporán de atención personalizada no horario de tutorías do profesor para a aclaración dos conceptos fundamentais da materia exposta nos grupos grandes, a resolución de cuestións individuais expostas nos seminarios e nas sesións maxistras. Ademais, o alumno poderá recibir atención personalizada sobre calquera aspecto da materia durante o horario de tutorías do profesor. |

Assessment

| Methodologies | Competencies | Description | Qualification |
|---------------------------------|---------------------------------|--|---------------|
| Problem solving | A1 A2 A3 B1 B2 B3 B7 B10 B11 | Continuous evaluation will count 40% in the grade for the course and consist of two components: interactive small group classes (seminars) and highly interactive small group classes (tutorials). Seminars and tutorials include the following problem solving and case studies (15%), writing papers and written (5%) reports, oral presentation [(case studies, problems), 10%] and oral questions during the course (10%). | 40 |
| Mixed objective/subjective test | A2 A3 B2 B3 B11 | The final exam will cover all the contents of the subject. | 60 |

Assessment comments

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Sources of information

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| Basic | <ul style="list-style-type: none"> - Hegedus, L. S.; Söderberg, B. C. G. (2009). Transition Metals in the Synthesis of Complex Organic Molecules 3rd Ed.. University Science Books - Bates, R. (2012). Organic Synthesis using Transition Metals. Wiley - Beller, M.; Bolm, C., Eds. (2004). Transition Metals for Organic Synthesis: Building Blocks and Fine Chemicals, 2nd Ed.. Wiley-VCH - De Meijere, A.; Diederich, F., Eds. (2004). Metal-Catalyzed Cross-Coupling Reactions, 2nd Ed.. Wiley-VCH - Crabtree, R. H.; Peris Fajarnés, E., Eds. (1997). Química organometálica de los metales de transición. Publicacions de la Universitat Jaume I |
| Complementary | |

Recommendations

Subjects that it is recommended to have taken before

Profundización en Química Orgánica/610509004
Profundización en Química Inorgánica/610509003



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| Subjects that are recommended to be taken simultaneously |
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| Análise Estrutural Avanzado/610509005 |
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| Mecanismos de reacción e catálise/610509009 |
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| Síntese estereoselectiva/610509012 |
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| Subjects that continue the syllabus |
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| Other comments |
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| (*)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. |
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