| Teaching Guide | | | | |
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| Identifying Data | | | | 2019/20 |
| Subject (*) | Applied Coordination Chemistry | | Code | 610509110 |
| Study programme | Mestrado Universitario en Investigación Química e Química Industrial (Plan 2017) | | | |
| Descriptors | | | | |
| Cycle | Period | Year | Type | Credits |
| Official Master's Degree | Yearly | First | Optional | 3 |
| Language | Spanish | | | |
| Teaching method | Face-to-face | | | |
| Prerequisites | | | | |
| Department | Química | | | |
| Coordinador | Fernandez Lopez, Alberto A. | E-mail | alberto.fernandez@udc.es | |
| Lecturers | Fernandez Lopez, Alberto A.<br>Platas Iglesias, Carlos | E-mail | alberto.fernandez@udc.es<br>carlos.platas.iglesias@udc.es | |
| Web | | | | |
| General description | Este curso enmárcase na especialidade de Química Sintética dedicado ao estudo da síntese e propiedades de diversas especies químicas. Dentro de dita especialidade escolléronse algúns tipos de compostos que, xa sexa polas súas especiais características, xa sexa polas súas aplicacións futuras, merecen un estudo detallado. Tendo isto en conta, a Química da Coordinación merece un estudo aparte, tanto polas particulares características dos compostos de coordinación como polos seus métodos de síntese. Desde outro punto de vista, os chamados complexos preséntanse nunha variedade estrutural enorme que vai desde especies de dimensión molecular pasando por agregados supramoleculares, polímeros mono-, bi-, e tridimensionáis, ata chegar ao chamados Metal Organic Frameworks (MOFs) que forman redes tridimensionáis ordenadas. Dada esta enorme variedade estrutural, non é de sorprender que o número de propiedades e aplicacións que presentan sexa tamén diverso. Todas estas razóns xustifican a súa inclusión tanto na especialidade de Química sintética como nun Máster dedicado ao estudo da Química. | | | |

| 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 |
| 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. |
| 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. |
| 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 |
| 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 |
| B12 | Being able to work in a team and adapt to multidisciplinary teams. |
| C1 | CT1 - Elaborar, escribir e defender publicamente informes de carácter científico e técnico |
| C3 | CT3 - Traballar con autonomía e eficiencia na práctica diaria da investigación ou da actividade profesional. |
| C4 | CT4 - Apreciar o valor da calidade e mellora continua, actuando con rigor, responsabilidade e ética profesional. |

| Learning outcomes |
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| Learning outcomes | Study programme competences / results | | |
|---|---|---|---|
| Students will be able to design new routes to prepare and isolate coordination compounds. | AC1<br>AC2<br>AC3<br>AC8 | BC1<br>BC2<br>BC3<br>BC4<br>BC7<br>BC10 | CC1<br>CC3 |
| Students will be able to identify the chirality in mononuclear coordination complexes and identify its origin | AC1<br>AC2<br>AC3<br>AC8 | BC1<br>BC2<br>BC3<br>BC7<br>BC10 | CC4 |
| Students will be able to describe the factors that imply activation small molecules after coordination to metal centres and their applications. | AC1<br>AC2<br>AC3<br>AC8 | BC1<br>BC2<br>BC3<br>BC7<br>BC10<br>BC12 | |

| Contents | |
|---|---|
| Topic | Sub-topic |
| Structural properties of coordination compounds. Characterization techniques | Structural properties in coordination compounds.<br>Characterization techniques.<br>- Spectroscopic techniques<br>- Spectrometric techniques<br>- Diffraction techniques<br>- Techniques based on magnetic properties<br>- Other techniques |
| Activation of small molecules by coordination compounds | Structure and bonding in dioxygen and dinitrogen complexes: bonding modes.<br>Synthesis of dioxygen and dinitrogen complexes.<br>Structural characterization of dioxygen and dinitrogen complexes: NMR and IR spectroscopy, mass spectrometry, single crystal X-ray diffraction.<br>Synthetic applications of dioxygen and dinitrogen complexes. Future perspectives. |
| Coordination compounds with applications in medicine: therapeutic and diagnose tools | Coordination compounds with applications in medicine: therapeutic and diagnose tools<br>- Antitumor metalodrugs.<br>- Types of complexes according to the metal centre and the structure<br>- Therapeutic mechanism.<br>- Synthetic methods.<br>Application of metal complexes as radiopharmaceuticals.<br>- Properties and characteristics of the ligands and the radioisotope<br>- Diagnostic, (PET, SPEC) and therapeutic techniques.<br>Contrast agents in magnetic resonance imaging (MRI)<br>Proton relaxation agents T1 (Gd3+, Mn2+ y Fe3+) y T2. Parameters affecting the efficiency.<br>- Agents based on saturation transfer by chemical exchange (CEST).<br>- Agents based on other nuclei (, 31P).<br>- Hyperpolarization. |

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| Coordination compounds in the design of new materials: coordination polymers and MOFs. Properties and applications. | Types of systems arising from the metal-ligand association. Isolated and extensive associations (coordination polymers and MOFs) Main structural characteristics and characterization.<br>Synthetic strategies and general characterization techniques.<br>Properties and applications. |

| Planning | | | | |
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| Methodologies / tests | Competencies / Results | Teaching hours (in-person & virtual) | Student?s personal work hours | Total hours |
| Seminar | A1 A2 A3 B1 B2 B3 B4 B7 B10 B12 C1 C3 C4 | 7 | 21 | 28 |
| Mixed objective/subjective test | A1 A2 A3 A8 B1 B10 | 2 | 18 | 20 |
| Guest lecture / keynote speech | A2 A3 B3 B7 B12 C4 | 12 | 13 | 25 |
| 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 | 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.) |
| Mixed objective/subjective test | Tests designed to gauge the achievement of both theoretical and practical knowledge and the acquisition of skills and attitudes. |
| Guest lecture / keynote speech | The lectures in which the contents of the subject will be explained with the assistance of illustrative examples. The class slides will be available, prior to the class.<br>In some cases, if the number of students and their characteristics are adequate complementary methodologies as, for example, the case study or analyses of bibliographic sources might be used. The active participation of students will be encouraged.<br>Attendance to lectures is not compulsory by highly advisable. |

| Personalized attention | |
|---|---|
| Methodologies | Description |
| Seminar<br>Mixed objective/subjective test | Individual or small group tutorials designed to support the students in the learning process. The student may attend to the tutorial freely to solve any doubts related to the subject. Tutorials are particularly important to solve the proposed problems or the assigned tasks.<br>Students granted the ?part time? condition will be given special attention through the tutorials which will be dedicated specifically to the solution of the problem sheets. |

| Assessment | | | |
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| Methodologies | Competencies / Results | Description | **Qualification** |
| Guest lecture / keynote speech | A2 A3 B3 B7 B12 C4 | Continuous assessment of students through questions made during the classes. Attendance and active participation will also be assessed | 10 |
| Seminar | A1 A2 A3 B1 B2 B3 B4 B7 B10 B12 C1 C3 C4 | Resolution of problems and study cases. Attendance will also be assessed as well as the active participation to de different activities. | 20 |

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| Mixed objective/subjective test | A1 A2 A3 A8 B1 B10 | Mixed test exam with questions and problems related to class contents. | 70 |

| Assessment comments |
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| The ?no presentado? mark will be granted to those students who do not attend to the mixed text.<br><br>Students granted the ?part time student? condition will be assessed exclusively by the mixed text marks (100% of the subject mark) |

| Sources of information | |
|---|---|
| Basic | - J. Rivas Gispert (2000). Química de Coordinación. Omega<br>- J. Rivas Gispert (2008). Coordination Chemistry . Weinheim: Willey-VCH |
| Complementary | - Patrick L. Holland. Metal?dioxygen and metal?dinitrogen complexes: where are the electrons? Dalton Trans. , 2010, 39 , 5415?5425. - Michael P. Shaver, Michael D. Fryzuk. Activation of Molecular Nitrogen: Coordination, Cleavage andFunctionalization of N2 Mediated By Metal Complexes. Adv. Synth. Catal.2003, 345 , 1061- 1076 - Hiromasa Tanaka, Yoshiaki Nishibayashi, and Kazunari Yoshizawa, Interplay between Theory and Experiment forAmmonia Synthesis Catalyzed by Transition Metal Complexes, Acc. Chem. Res.2016, 49, 987?995.- Serenella Medici, Massimiliano Peana,Valeria Marina Nurchi, Joanna I. Lachowicz,Guido Crisponi, Maria AntoniettaZoroddu. Noble metalsin medicine: Latest advances. CoordinationChemistry Reviews, 2015, 284, 329?350.- A. Merbach, L. Helm and E. Tóth, The Chemistry of Contrast Agents inMedical Magnetic Resonance Imaging: Second Edition , John Wiley & Sons,Chichester, 2013. - Eric W. Price and Chris Orvig. Matchingchelators to radiometals for radiopharmaceuticals. Chem. Soc. Rev., 2014, 43,260-290.- - Stuart R. Batten, Neil R. Champness, Xiao-MingChen, Javier Garcia-Martinez, Susumu Kitagawa, Lars Öhrström, MichaelO?Keeffe7, Myunghyun Paik Suh, and Jan Reedijk. Terminology of metal?organic frameworks andcoordination polymers (IUPAC Recommendations 2013) . Pure Appl. Chem., 2013, 85, 1715?1724. - - Bradley J. Holliday and Chad A. Mirkin, Strategies for the Construction of Supramolecular Compounds throughCoordination Chemistry , Angew. Chem. Int. Ed. 2001, 40, 2022-2043. - Shin-ichiroNoro, Hitoshi Miyasaka, Susumu Kitagawa, Tatsuo Wada,Takashi Okubo, MasahiroYamashita, and Tadaoki Mitani. FrameworkControl by a Metalloligand Having Multicoordination Ability: New SyntheticApproach for Crystal Structures and Magnetic Properties . Inorg.Chem. 2005, 44, 133-146. |

| Recommendations |
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| Subjects that it is recommended to have taken before |
| /<br>Advanced Structural Determination/610509103 |
| Subjects that are recommended to be taken simultaneously |
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| Subjects that continue the syllabus |
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| Other comments |
| The student must know the basic principles of coordination chemistry as, for example, the definition of coordination compound and its components, as well as the bonding theories used to describe this type of compounds |

(*)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.