



## Teaching Guide

| Teaching Guide           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |        |                     |           |
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| Identifying Data         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |        |                     | 2017/18   |
| Subject (*)              | Elucidation of Reaction Mechanisms                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |        | Code                | 610500013 |
| 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  | Optativa            | 3         |
| Language                 | SpanishGalicianEnglish                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |        |                     |           |
| Teaching method          | Face-to-face                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |        |                     |           |
| Prerequisites            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |        |                     |           |
| Department               | Química                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |        |                     |           |
| Coordinador              | Canle López, Moisés                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | E-mail | moises.canle@udc.es |           |
| Lecturers                | Canle López, Moisés                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | E-mail | moises.canle@udc.es |           |
| Web                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |        |                     |           |
| General description      | <p>The contents of the subject "Elucidation of Reaction Mechanisms" are oriented to complement previous knowledge from the graduation studies. Usually, reaction mechanisms are proposed for chemical processes without any indication of the experimental evidences that lead to such mechanism instead of any other. This subject will show which are such evidences and how they can be obtained.</p> <p>It is not frequent to face the planification of a research into how chemical reactions take places. This subject will face this kind of problem from a practical point of view. There are a number of techniques, direct and indirect evidences that allow the elucidation of the mechanism of a chemical process.</p> <p>Chemical reactivity is central to changes in nature, and the recognition of the different reaction mechanisms is fundamental to control chemical process, from the kinetic, thermodynamic points of view or even from the point of view of the generated products.</p> |        |                     |           |

## 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.                                                                                                                                     |
| 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 tecnolóxica.                                                                                |
| A6   | Coñecemento do comportamento de diferentes especies químicas e dos procesos aos que poden estar sometidas unha vez liberadas no medio ambiente, incluíndo as súas relacións entre distintos compartimentos ambientais.                                                                 |
| A7   | Coñecer o marco teórico e as aplicacións da electroquímica e da fotocatalise nos campos da enerxía e o medio ambiente.                                                                                                                                                                 |
| A8   | Coñecer os fundamentos das interaccións intermoleculares e as súas aplicacións no campo da catalise supramolecular, recoñecemento molecular e biocatalise.                                                                                                                             |
| A9   | Coñecer algunhas aplicacións básicas da química computacional e dos programas de cálculo máis utilizados nos ámbitos da química e o medio ambiente.                                                                                                                                    |
| A11  | Coñecer as distintas técnicas experimentais e computacionais orientadas á caracterización de mecanismos de reacción.                                                                                                                                                                   |
| A20  | Coñecemento dos principais tipos de produtos naturais: enzimas, receptores moleculares, etc. Entender a súa participación en procesos de catalise e autoensamblaxe.                                                                                                                    |
| A22  | Dominar as técnicas instrumentais de análises máis típicas no ámbito químico profesional.                                                                                                                                                                                              |
| 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 coñecidas 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 xuízos. |
| 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.                                                                                                 |
| B5  | Que os estudantes posúan as habilidades de aprendizaxe que lles permitan continuar estudando dun modo que haberá de ser en gran medida autodirixido ou autónomo.                                                                                                                             |
| B6  | Ser capaz de analizar datos e situacións, xestionar a información dispoñible e sintetizala, todo iso a un nivel especializado.                                                                                                                                                               |
| B7  | Ser capaz de planificar adecuadamente desenvolvementos experimentais, a un nivel especializado.                                                                                                                                                                                              |
| C1  | Ser capaz de traballar en equipos, especialmente nos interdisciplinares e internacionais.                                                                                                                                                                                                    |
| C2  | Ser capaz de manter un pensamento crítico dentro dun compromiso ético e no marco da cultura da calidade.                                                                                                                                                                                     |
| C3  | Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado.                                                                                                                                                                |
| C4  | Expresarse correctamente, tanto de forma oral coma escrita, nas linguas oficiais da comunidade autónoma.                                                                                                                                                                                     |
| C5  | Dominar a expresión e a comprensión de forma oral e escrita dun idioma estranxeiro.                                                                                                                                                                                                          |
| C9  | Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben enfrontarse.                                                                                                                                                            |
| C10 | Asumir como profesional e cidadán a importancia da aprendizaxe ao longo da vida.                                                                                                                                                                                                             |
| 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             |                                 |                                                 |
| To go deeper into the physical basis of chemical reactivity.                                                                     | AC4<br>AC6<br>AC7<br>AC8<br>AC9<br>AC20 | BC1<br>BC2                      | CC1<br>CC3<br>CC9<br>CC11                       |
| To expand the knowledge and ability to use experimental techniques to determine and measure chemical reactivity and its changes. | AC11<br>AC22                            | BC7                             |                                                 |
| To understand the different concepts and theories necessary to characterize chemical processes and their course.                 | AC4<br>AC7<br>AC9                       | BC2<br>BC3<br>BC6               | CC1<br>CC3<br>CC9<br>CC11                       |
| To be able to use different instruments that are frequently used for the characterization of reaction mechanisms.                | AC9<br>AC11<br>AC22                     | BC3<br>BC7                      | CC3                                             |
| To be able to use / apply acquired abilities and concepts for the resolution of practical examples..                             | AC1<br>AC3<br>AC4<br>AC6                | BC2<br>BC3<br>BC4<br>BC5<br>BC6 | CC2<br>CC3<br>CC4<br>CC5<br>CC9<br>CC10<br>CC11 |

| Contents       |                                                                                               |
|----------------|-----------------------------------------------------------------------------------------------|
| Topic          | Sub-topic                                                                                     |
| Reaction media | Variables that influence chemical processes.<br>Role of reaction medium in chemical processes |



|                                                                    |                                                                                                                                   |
|--------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| Reaction mechanisms                                                | Classification of reaction mechanisms<br>Kinetic and thermodynamic characteristics of the main reaction mechanisms                |
| Experimental techniques for the elucidation of reaction mechanisms | Batch methods<br>Continuous methods<br>Techniques for the study of rapid and ultrarapid reactions                                 |
| Chemical reactivity                                                | Catalysis<br>Kinetic isotope effects<br>Linear free energy relationships (LFER) and quantitative structure-activity relationships |
| Photochemistry                                                     | General concepts<br>Photochemical processes<br>Photochemistry and photoreactivity                                                 |

| Planning                                                                                                                        |                                               |                      |                               |             |
|---------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------|----------------------|-------------------------------|-------------|
| Methodologies / tests                                                                                                           | Competencies                                  | Ordinary class hours | Student's personal work hours | Total hours |
| Guest lecture / keynote speech                                                                                                  | A1 A4 A6 A7 A8 A9<br>A11 A20 A22 B1 B5<br>C10 | 10                   | 20                            | 30          |
| Case study                                                                                                                      | A3 B2 B3 B4 B6 B7<br>C2 C3 C4 C5 C9 C11       | 4                    | 6                             | 10          |
| Laboratory practice                                                                                                             | B2 B4 B6 C1 C4 C5                             | 15                   | 18.75                         | 33.75       |
| Objective test                                                                                                                  | A4 A6 A7 A8 A9 A11<br>A20 A22 B2 B3 B4 B6     | 1                    | 0                             | 1           |
| 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 | ? Two-hour sessions to present the masterlines of the subject, indicating the students the most relevant points to take into account when studying and recommending appropriate materials for a better comprehension.<br>? The students will have the audiovisual material available through the Moodle virtual platform. |
| Case study                     | ? Different real cases will be critically analyzed and discussed, in order to apply the acquired knowledge                                                                                                                                                                                                                |
| Laboratory practice            | ? Will take place in the laboratory, in the days and hours that will be announced.<br>? At the end of the practical lessons, the student will hand a report on the experimental project developed, and realize a short oral presentation analyzing the experimental part and the meaning of the obtained results.         |
| Objective test                 | ? There will be a short exam, that may include both theory and practice                                                                                                                                                                                                                                                   |

| Personalized attention            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|-----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Methodologies                     | Description                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| Case study<br>Laboratory practice | Will be carried out at the lecturers' offices, or at the Laboratory of Physical Chemistry I, according to the established timetable (consult for each lecturer).<br>Proposed exercises, laboratory reports, etc. may be hand directly in these hours, solving any doubt or question about them.<br>Doubt or questions with a simple and brief answer may be asked and answered through the Moodle virtual platform. More complicated topics will need an appointment. |

| Assessment |
|------------|
|------------|



| Methodologies       | Competencies                              | Description                                                                                                                        | Qualification |
|---------------------|-------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|---------------|
| Case study          | A3 B2 B3 B4 B6 B7<br>C2 C3 C4 C5 C9 C11   | Evaluation will be centered in the critical analysis of the proposed cases, as well as on the suggestion of alternative solutions. | 20            |
| Objective test      | A4 A6 A7 A8 A9 A11<br>A20 A22 B2 B3 B4 B6 | May include short test or multiple choice questions or short problems / cases to analyze.                                          | 40            |
| Laboratory practice | B2 B4 B6 C1 C4 C5                         | Both the experimental design and the critical analysis of the obtained results will be evaluated.                                  | 40            |
| Others              |                                           |                                                                                                                                    |               |

#### Assessment comments

Para superar la asignatura habrá que asistir tanto a las prácticas de laboratorio como a las simulaciones.

#### Sources of information

|               |                                                                                                                                                                                                                                                                                                                                                                                                   |
|---------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Basic         | <ul style="list-style-type: none"><li>- H. Maskill (1985). The Physical Basis of Organic Reactivity. Oxford University Press</li><li>· Study materials or reference to them will be accesible through the Moodle virtual platform.</li></ul>                                                                                                                                                      |
| Complementary | <ul style="list-style-type: none"><li>- H. Maskill (Ed.), (2006 ). Investigating Organic Reaction Mechanisms . Blackwell Science</li><li>- N. J. Turro; V. Ramamurthy; J.C. Scaiano (2009). Principles of Molecular Photochemistry. An Introduction. University Science Books</li><li>- E.V. Anslyn, D.A. Dougherty (2006). Modern Physical Organic Chemistry. University Science Books</li></ul> |

#### 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

A higher profit from this subject would require actualized knowledge of Physical Chemistry. It is strongly recommended to review the theoretical concepts introduced in the lessons through the resolution of questions and exercises, that will be proposed.

(\*)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.