

**COURSE DATA****Data Subject**

<b>Code</b>	44612
<b>Name</b>	Advanced characterisation of chemicals
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	5.0
<b>Academic year</b>	2019 - 2020

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2218 - M.U. en Química	Faculty of Chemistry	1	Second term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2218 - M.U. en Química	7 - Advanced characterisation of chemicals	Optional

**Coordination**

<b>Name</b>	<b>Department</b>
GIMENO ADELANTADO, JOSE VICENTE	310 - Analytical Chemistry

**SUMMARY**

The subject *Advanced Characterization of Chemical Substances* is an optional subject of the academic (or research) itinerary, mainly intended to provide students with in-depth knowledge and contents complementary to those acquired in the core subject *Advanced Chemistry*, especially in advanced techniques for characterization of chemicals from an interdisciplinary perspective. The subject covers more deeply the study of techniques of special interest in chemical characterization that, due to their complexity and/or specialization level, had not been studied neither in the degree nor in the core subject *Advanced Chemistry*. Thus, the techniques to be covered are NMR and EPR, mass spectroscopy, X-ray based techniques, electrochemical techniques and others, as well as techniques specifically used in surface analysis (microscopic techniques TEM and SEM, XPS, microanalysis). In each case the fundamentals, methodological aspects and instrumentation as well as the main applications will be considered.



## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

### Other requirements

Prior knowledge of chemistry is required, at the level taught in the qualifications listed in the recommended profile for admission of candidates to the Masters Degree.

## OUTCOMES

### 2218 - M.U. en Química

- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Possess the necessary skills to develop multidisciplinary activities within the field of chemistry at the master's level.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.
- Acquire the necessary advanced knowledge to assess the importance of chemistry in economic and social development in a context of specialization.

## LEARNING OUTCOMES

- To learn the fundamentals of the main advanced instrumental techniques and their applications.
- To compare the different techniques according to their features and to select the most appropriate one according to the aim of the analysis or characterization and the required quality parameters
- To apply the data delivered by NMR spectroscopy, mass spectroscopy, X ray diffraction..., to elucidate the structure of chemical substances and intermolecular interactions.



## DESCRIPTION OF CONTENTS

### 1. Magnetic resonance spectroscopic techniques

Basics of advanced multidimensional Nuclear Magnetic Resonance (NMR), both homo and heteronuclear for the structural determination of complex organic molecules, organometallic compounds and biomacromolecules. NMR techniques applied to complex chemical systems: tissues, cells and biofluids.

### 2. X-Ray diffraction and fluorescence

Crystal symmetry. Space groups. International tables of crystallography. Nature of the X-Rays. Interference and Diffraction. Braggs law. Diffraction and crystalline structure. Resolution and refinement of crystalline structures (single-crystal). Molecular crystals and determination of intermolecular interactions and supramolecular assembly in the solid state. Determination of absolute configuration. Databases. X-ray fluorescence. Other related techniques: diffraction on polycrystalline samples, neutron diffraction.

### 3. Mass spectrometry

Inorganic and organic mass spectrometry. Fragmentology. Instrumental components. Hybridization with chromatographic techniques. Working modes in low and high resolution hybridization. Examples of applications. Isotopic analysis by mass spectrometry.

### 4. Surface techniques

Electron microscopy (SEM, TEM and high resolution). Spectroscopy of electrons. Applications.

### 5. Other techniques

Electrochemical techniques: microparticle voltammetry and impedance techniques.

**WORKLOAD**

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	5,00	100
Seminars	5,00	100
Study and independent work	75,00	0
<b>TOTAL</b>	<b>125,00</b>	

**TEACHING METHODOLOGY**

The course will be taught using participatory classes, seminars aimed at resolving practical problems, and tutorials in which the ability of the students to understand the different topics covered will be evaluated. Additionally, the Aula Virtual platform will be used for communication and information exchange.

**EVALUATION****First call:**

The score in the first call will be calculated from the scores obtained in a final examination and the continuous assessment of each student-based activities students along the course. The final grade will be calculated according to the following percentages:

- (a) Final exam: 70%.
- (b) Continuous assessment: 30%.

The score on each of these two parts must be at least 4.5 in order to apply the average.

The minimum overall grade to pass the course is 5.0.

**Second call:**

In the second call the final grade will be obtained by applying the same criteria as in the first call.

**REFERENCES****Basic**

- Duddeck H., Dietrich W. y Tóth G.; Elucidación estructural por RMN, Springer, 2000. (traducción de la 3ª edición revisada y ampliada) (ISBN 8407005053)



- Simpson, J. H., Organic Structure Determination Using 2-D NMR Techniques. A Problem Based Approach, 2nd Ed., Academic Press, 2012. (ISBN :9780123849700)
- Hammond, C. The basics of Crystallography and Diffraction. Oxford University Press (IUCr Texts in Crystallography, 12) Third edition, 2009
- Massa, W. Crystal structure determination. Springer-Verlag, 2004
- Jenkins, R. X-ray fluorescence spectrometry. 2nd. edition, Wiley, 1999
- Ríos Castro, A.; Moreno Bondi, M. C.; Simonet Suau, B. M. (Coords.) Técnicas espectroscópicas en química analítica (vol. I y II), Síntesis S. A., Madrid, 2012.
- Goldstein, J.I.; Newbury, D.E.; Echlin, P.; Joy, D.C.; Fioril, Ch.; Lifshin, E. Scanning Electron Microscopy and X-Ray Microanalysis. Plenum Press, Nueva York, 1984.
- Bonnel, D.A. (Ed.) Scanning Probe Microscopy and Spectroscopy: Theory, Techniques and Applications. 2ª ed., Wiley, Nueva York, 2001.
- Watts J. F, Wolstenholme J. An introduction to surface analysis by XPS and AES. Wiley, Chichester, 2008.
- Taylor H.E., Inductively Coupled Plasma-Mass Spectrometry. Practices and Techniques, Academic Press, San Diego, 2001
- Desiraju G.R., Vittal, J.J., Ramanan, A.; Crystal Engineering: A Textbook, World Scientific Publishing Company, 2011.
- Desiraju, G.R.; Crystal Engineering: The Design of Organic Solids, Elsevier, 1989.
- Müller, P. et al. Crystal Structure Refinement (A crystallographer's guide to SHELXL). IUCr Oxford Science Publications, 2006

#### **Additional**

- Pretsch, E.; Bühlmann, P.; Affolter, C.; Herrera, A., Determinación estructural de compuestos orgánicos, Masson, 2002. (ISBN: 9788445812150)
- Friebolin H.; Basic One- and Two-Dimensional NMR Spectroscopy, 5th, Completely Revised and Updated Edition, Wiley-VCH, 2010.  
ISBN: 978-3-527-32782-9
- Hühl, O.; Phosphorus-31 NMR Spectroscopy. A Concise Introduction for Synthetic Organic and Organometallic Chemist, Springer, 2008 (ISBN: 9783540791171)
- Hesse, M.; Meier, H.; Zehe, B., Métodos espectroscópicos en Química Orgánica, (traducción de la 5ª edición de la versión en alemán), 2ª ed. Síntesis, 1999 . (ISBN:847738522X)
- The Cambridge Structural Database (CSD), Comprehensive of the published literature and highly curated, is an essential resource to scientists around the world.
- Mercury - Crystal Structure Visualisation, Exploration and Analysis Made Easy





- Doménech, A.; Doménech, M.T.; Costa, V. Electrochemical methods for archaeometry, conservation and restoration, Springer, Berlin, 2009.
- Doménech, A. Electrochemistry of Porous Materials, Taylor & Francis, Boca Raton, 2010.
- International Tables for Crystallography, Vol. A, 2006 (Space-group symmetry) + Vol A1, 2011 (Symmetry relations between space groups)
- Lifshin, E. (editor) X-ray Characterization of Materials. Wiley-VCH, 1999

## **ADDENDUM COVID-19**

**This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council**

### **1. Contents**

The contents initially collected in the teaching guide are maintained.

Prior to March 13, 22 face-to-face sessions had been taught out of a total of 24, which means 91.7% of teaching. The remaining 2 sessions have been taught online.

### **3. Volume of work and temporary planning of teaching**

Workload and time planning are maintained on scheduled days and times.

### **3. Teaching methodology**

The teaching methodology indicated in the teaching guide is maintained. The face-to-face teaching is replaced by: Study of the material provided by the teachers in the Virtual Classroom, synchronous videoconferences, resolution of doubts in forums and email.

### **4. Evaluation**

The weight of this subject will be maintained in accordance with the provisions of the original teaching guide.

A) Exam: 70%

B) Continuous evaluation actions: 30%

In the case of not being able to make an in-person evaluation, the exams of the first and second calls will be carried out online using the means available for it.



## 5. Bibliography

The bibliography described to the students in the Teaching Guide is maintained. To this bibliography we must add the material that the teachers had uploaded to the Virtual Classroom. Students who do not have the books can access the Library Service online.