VNIVERSITAT DE VALÈNCIA

Course Guide
44612 Advanced characterisation of chemicals

COURSE DATA

Data Subject	
Code	44612
Name	Advanced characterisation of chemicals
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2018 - 2019

Study (s)

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

Subject-matter

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

Coordination

Name	Department
GIMENO ADELANTADO, JOSE VICENTE	310 - Analytical Chemistry

SUMMARY

The subject *Advanced Characterization of Chemical Substances* is an optional subject of the academic and research, 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 chemical substances from an interdisciplinary perspective. The subject covers more deeply the study of techniques of special interest in chemical characterization that, because of 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

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.

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
TOTAL	**125,00**	

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 3º 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.; FioriI, 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.; Zeeh, 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