27219 - Structure Determination

Información del Plan Docente

Academic Year	2017/18
Faculty / School	100 - Facultad de Ciencias
Degree	452 - Degree in Chemistry
ECTS	6.0
Year	4
Semester	First semester
Subject Type	Compulsory
Module	---

1.General information

1.1.Introduction

1.2.Recommendations to take this course

1.3.Context and importance of this course in the degree

1.4.Activities and key dates

2.Learning goals

2.1.Learning goals

2.2.Importance of learning goals

3.Aims of the course and competences

3.1.Aims of the course

3.2.Competences

4.Assessment (1st and 2nd call)

4.1.Assessment tasks (description of tasks, marking system and assessment criteria)

5.Methodology, learning tasks, syllabus and resources

5.1.Methodological overview

The learning process that has been designed for this subject is based on the following:

1.- Lectures, in which the teacher will explain the theoretical foundations of the different techniques and how they are applied for the structural determination.

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2.- Resolution and discussion of problems and cases. Typical problems include those in which students will be asked to use the concepts learned in order to deduce the structure compatible with the spectroscopic data given or to propose the expected spectrum for a known molecule.

3. Demonstrations, related to the preparation of samples and the measurement of the spectroscopic properties of selected compounds.

Students are encouraged to participate and discuss different aspects of the subject in order to develop critical thinking and inquiry-based learning.

5.2.Learning tasks

The learning program includes the following activities

1. Lectures (30 sessions of 50 min, 3 ECTS).
2. Problem resolution, case studies and demostrations (30 sessions of 50 min, 3 ECTS).

5.3.Syllabus

- Characterization of chemical compounds: general aspects.
- Infrared spectroscopy. Bases and applications. Types of vibrations. Regions of the IR spectrum. Study of the functional groups. Interpretation of spectra. Problems and case studies. Instrumentation. Sample preparation.
- Mass spectrometry. Bases and applications. Ionization methods and ions analysis. Molecular ion. Isotopic peaks. Mass exact. Fragmentations. Problems and case studies. Instrumentation. Sample preparation.
- Nuclear magnetic resonance: proton. Bases and applications. Instrumentation. Chemical shift and shielding. Chemical equivalence. Integration. Spin-spin coupling. Study of the functional groups. Handling of the data tables. Problems and case studies. Sample preparation.
- Nuclear magnetic resonance: carbon. Bases and applications. Study of the functional groups. Handling of the data tables. Two-dimensional NMR. Problems and case studies.
- Strategies for the assignment of the structure of a compound from the corresponding spectra.
- Nuclear magnetic resonance of other nuclei. Nuclei with different nuclear spin and different isotopic abundance. Satellites. Spin systems. Problems and case studies.
- Nuclear magnetic resonnace spectra of first and second order. Chemical and magnetic inequivalence. Simplification of spectra. Fluxionality in chemical compounds. Problems and case studies.
- UV-visible spectroscopy. Chromophores of general interest. Electronic spectra: types of transitions. Transitions in the free ion and in complex ions. Splitting of the d orbitals: strong-field and weak field approximations. Correlation diagrams. Tanabe-Sugano diagrams. Selection rules. Jahn-Teller effect. Problems and case studies.
- Magnetic susceptibilities in transition metal complexes. Effective magnetic moment. Orbital contribution. Problems and case studies.

5.4.Course planning and calendar

The schedule of sessions is published in the bulletin board and web page of the Faculty of Science (http://ciencias.unizar.es/web/horarios.do)

There will be two partial examinations, whose exact dates will be communicated well in advance on the bulletin board and through the ADD. As a guide, the examinations will take place in early December and in mid-January.

5.5.Bibliography and recommended resources

BB	Determinación estructural de compuestos orgánicos / E. Pretsch ... [et al.] . - Reimp.

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	Barcelona [etc.] : Masson, 2005
BB	Hesse, Manfred. Métodos espectroscópicos en química orgánica / Manfred Hesse, Herbert Meier, Bernd Zeeh ; adaptación española 2ª edición, Antonio Herrera Fernández, Roberto Martínez Álvarez . 2ª ed. act. y amp. Madrid : Síntesis, D.L. 2005
BB	Pretsch, E.. Structure determination of organic compounds. Tables of spectral data. 4th revised and enlarged Springer 2001
BB	Requena Rodríguez, Alberto. Espectroscopía / Alberto Requena Rodríguez, José Zúñiga Román Madrid [etc.] : Pearson/Prentice Hall, cop. 2004
BB	Roberts, John D. ABCs of FT-NMR / John D. Roberts Sausalito, California : University Science Books, cop. 2000
BB	Silverstein, Robert M.. Spectrometric identification of organic compounds / Robert M. Silverstein, G. Clayton Bassler, Terence C. Morrill . - 4th ed. New York [etc.] : Wiley, cop. 1981
BC	Duckett, Simon. Foundations of spectroscopy / Simon Duckett and Bruce Gilbert . - 1st published, repr. Oxford [etc.] : Oxford University Press, 2004
BC	Ebsworth, E. A. V. Structural methods in inorganic chemistry / E.A.V. Ebsworth, David W.H. Rankin, Stephen Cradock ; foreword by Kenneth Raymond . - 2nd ed. Oxford [etc.] : Blackwell, 1991
BC	Harwood, Laurence M..Introduction to organic spectroscopy / Laurence M. Harwood, Timothy D. W. Claridge . - 1st publi., repr. Oxford : Oxford University Press, 2007

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Online resources:

Organic Structure Elucidation. A Workbook of Unknowns - [http://www3.nd.edu/~smithgrp/structure/workbook.html]

WebSpectra. Problems in NMR and IR Spectroscopy - [http://www.chem.ucla.edu/~webspectra/]

Complementary material: exercises, questions, presentations, etc. will be available to students in reprography and in the website https://moodle2.unizar.es/add/.