27219 - Structure Determination

Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	452 - Degree in Chemistry
ECTS	6.0
Course	4
Period	First semester
Subject Type	Compulsory
Module	---

1.Basic info

1.1.Recommendations to take this course

1.2.Activities and key dates for the course

2.Initiation

2.1.Learning outcomes that define the subject

2.2.Introduction

3.Context and competences

3.1.Goals

3.2.Context and meaning of the subject in the degree

3.3.Competences

3.4.Importance of learning outcomes

4.Evaluation

5.Activities and resources

5.1.General methodological presentation

5.2.Learning activities

5.3.Program

- 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.

27219 - Structure Determination

- 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.Planning and scheduling

5.5.Bibliography and recomended resources

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

27219 - Structure Determination

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

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/]