

27221 - Spectroscopy and Molecular Properties

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 methodology followed in this course is oriented towards achievement of the learning objectives.

- Formative activity 1: Lecture classes (3.1 ECTS)

- Formative activity 2: problem‐solving sessions (1.5 ECTS)

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- Formative activity 3: laboratory sessions (1.4 ECTS)

Students are expected to participate actively in the class throughout the semester. In laboratory sessions, special attention will be paid to the understanding of the instrumental part and to the development of the skills and attitudes needed for the work in the laboratory.

Classroom materials will be available via Moodle. Further information regarding the course will be provided on the first day of class.

5.2. Learning tasks

The course includes 6 ECTS organized according to:

- Molecular symmetry (0.9 ECTS): 9 hours (6 h theory; 3 h problems).
- Photochemistry (0.5 ECTS): 5 hours (3 h theory; 2 h problems).
- Molecular spectroscopy (3.5 ECTS): 25 hours (17 h theory; 8 h problems) + 10 hours of laboratory (3 sessions).
- Polymers (1.1 ECTS): 7 hours (5 h theory; 2 h problems) + 4 hours of laboratory (1 session).

5.3. Syllabus

1. Molecular symmetry:

- * Introduction to molecular symmetry and group theory.
- * Symmetry operations and symmetry elements. Symmetry classification of molecules in point groups.
- * Irreducible representations and symmetry species. Character tables. Direct products of irreducible representations. Selection rules in spectroscopy.
- * Application of symmetry concepts to the study of normal modes of vibration and molecular orbitals.

2. Photochemistry:

- * Introduction to photochemistry.
- * Properties of molecules in excited electronic states. Overview of deactivation processes. Jablonski diagrams.
- * Basic photochemical reactions.

3. Molecular spectroscopy:

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- * Basic principles in spectroscopy; interaction between electromagnetic radiation and matter. Transition moment. Selection rules. Width of spectroscopic signals.
- * Rotational spectroscopy. Energy levels of molecules considered as rigid rotors. Centrifugal distortion constants. Stark effect in rotational spectroscopy.
- * Vibration in diatomic molecules; anharmonicity. Normal modes of vibration in polyatomic molecules. Characteristic group frequency in IR spectroscopy.
- * Raman effect. Vibrational and rotational Raman spectra. Light polarization in Raman effect. Application of IR and Raman spectra to the structure determination of molecules.
- * Electronic spectroscopy of diatomic molecules. Frank-Condon principle. Electronic spectroscopy of polyatomic molecules. Characteristics and applications of transitions in UV-vis.
- * Fluorescence spectroscopy: basic principles and applications.
- * Fundamentals of photoelectron spectroscopy. Interpretation of UPS and XPS spectra.
- * Resonance spin spectroscopy; Larmor precession. ¹H-NMR spectroscopy. Chemical shift and coupling constant. Analysis of NMR spectra of nuclei other than ¹H; nuclear quadrupole relaxation.
- * Fundamentals of electron spin resonance spectroscopy ESR. Analysis of hyperfine structure in some examples.

4. Polymers:

- * Physicochemical properties and characterization of polymers.
- * Kinetics and mechanisms of polymerization.
- * Degradation and stability.
- * Solubility of polymers.

5.4.Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course please refer to the Faculty website (<http://ciencias.unizar.es/web/horarios.do>).

5.5.Bibliography and recommended resources

BB

Banwell, C. N. : Fundamentals of
molecular spectroscopy / Colin N. Banwell,

27221 - Spectroscopy and Molecular Properties

Elaine M. McCash . - 4rth ed. London [etc.]
: McGraw-Hill, cop. 1994

- BB** Barrow, Gordon M.. Introduction to molecular spectroscopy / Gordon M. Barrow. - International student ed., 16th print. Auckland [etc] : McGraw-Hill, 1986
- BB** Chang, Raymond. Principios básicos de espectroscopía / Raymond Chang ; traducción I.Katime Amashta . - [1a. ed. española] Madrid : AC, D.L. 1983
- BB** Cotton, Frank Albert. La teoría de grupos aplicada a la química / F. Albert Cotton ; [versión española, Francisco de Asis Gonzales Vilchez ; revisión, Jaime Keller Torres] . - 2a. ed., [1a. reimp.] México, D.F. : Limusa, 1983
- BB** Drago, Russell S.. Physical methods for chemists. 2nd. Saunders College Pub. 1992
- BB** Levine, Ira N.. Espectroscopía molecular / Ira N. Levine ; [traducción, A. Fuster Ortigosa, A. Requena Rodríguez] . - [1a. ed. española] Madrid : Editorial AC, cop.1980
- BB** Polímeros / Javier Areizaga...[et. al.] Madrid : Síntesis , D.L. 2002
- BB** Walton, Paul H.. Beginning group theory for chemistry / Paul H. Walton Oxford [etc] : Oxford University Press, 1998
- BB** Wayne, Carol E.. Photochemistry / Carol E. Wayne and Richard P. Wayne . - Repr. with corr. Oxford [etc.]: Oxford University Press, 2002
- BC** Katime Amashta, Issa A.. Química física macromolecular / Issa A. Katime Bilbao : Universidad del Pais Vasco, Servicio Editorial, 1994
- BC** Requena Rodríguez, Alberto. Espectroscopía / Alberto Requena

27221 - Spectroscopy and Molecular Properties

Rodríguez, José Zúñiga Román Madrid
[etc.] : Pearson/Prentice Hall, cop. 2004

BC

Turro, Nicholas John. Modern molecular
photochemistry / Nicholas J. Turro Mill
Valley, California : University science
books, 1991

BC

Willcock, David J.. Molecular symmetry /
David J. Willcock Chichester : Wiley, 2009