

## 27221 - Spectroscopy and Molecular Properties

### 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

##### 1. Molecular symmetry: 9 hours (6 h theory; 3 h problems)

- Introduction to molecular symmetry and group theory.
- Symmetry operations and symmetry elements. Symmetry classification of molecules in point groups.

## 27221 - Spectroscopy and Molecular Properties

- 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: 5 hours (3 h theory; 2 h problems)

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

### 3. Molecular spectroscopy: 25 hours (17 h theory; 8 h problems) + 10 hours of laboratory (3 sessions).

- 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. <sup>1</sup>H-NMR spectroscopy. Chemical shift and coupling constant. Analysis of NMR spectra of nuclei other than <sup>1</sup>H; nuclear quadrupole relaxation.
- Fundamentals of electron spin resonance spectroscopy ESR. Analysis of hyperfine structure in some examples.

### 4. Polymers: 7 hours (5 h theory; 2 h problems) + 4 hours of laboratory (1 session).

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

### 5.4.Planning and scheduling

### 5.5.Bibliography and recommended resources

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

## 27221 - Spectroscopy and Molecular Properties

- 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 País Vasco, Servicio Editorial, 1994
- BC** Requena Rodríguez, Alberto. Espectroscopía / Alberto Requena 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** Willock, David J.. Molecular symmetry / David J. Willock Chichester : Wiley, 2009