Espectroscòpia 2014/2015

Code: 102531
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Química	OB	2	2

Contact

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Use of languages

Principal working language: anglès (eng)
Some groups entirely in English: Yes
Some groups entirely in Catalan: No
Some groups entirely in Spanish: No

Objectives and Contextualisation

In the topic of Spectroscopy the focus is the study of the interaction of electromagnetic radiation and matter, and how this interaction can be used to determine details on the structure of the latter. The theoretical foundations that explain the interaction of radiation and matter and predict the structured form of spectra are laid out first, relying on a working knowledge of quantum chemistry. Laser radiation is discussed, as its use is ubiquitous in current spectroscopic techniques. From there on, different spectroscopic techniques are discussed. For each kind, the structure of the corresponding spectrum is connected to the structural parameters of the molecules using quantitative relations derived from quantum mechanics. A specific focus is made on symmetry as a powerful tool to explain characteristics of certain spectra in polyatomic molecules.

Specific goals of the topic:

- Understand the basics of interaction of electromagnetic radiation with matter.
- Understand the rules that determine the frequency and intensity of a transition.
- Know how to apply this knowledge to be able to solve problems both in qualitative and quantitative aspects.

Content

Theory:

1. Introduction to Spectroscopy.

   Nature of the electromagnetic radiation. Electromagnetic spectrum. Spectroscopic techniques. Spectral line width. Uncertainty principle. Intensity of spectral lines. Selection rules. Raman Spectroscopy. Example: Rotational spectroscopy of diatomic molecules. Lasers.

2. Vibrational Spectroscopy.

   Vibration of diatomic molecules. Harmonic oscillator model. Anharmonicity. Dissociation energy. Rovibrational Spectra. Polyatomic molecules and Symmetry. Symmetry elements and operations. Symmetry point groups. Systematic determination of molecular point group. Vibration of polyatomic molecules: Normal modes of vibration. Types of normal modes. Symmetry of normal modes. Reducible and irreducible representations. Character tables. Selection rules for polyatomic molecules. Mutual exclusion rule.

3. Electronic Spectroscopy.

   Atomic spectroscopy. Spectral terms. Selection Rules. Electronic spectroscopy of diatomic molecules. Vibrational structure: vibronic spectra. Franck-Condon principle. Electronic spectroscopy of polyatomic molecules. Symmetry considerations. Fluorescence and phosphorescence. Photoelectron spectroscopy.

4. Magnetic Resonance Spectroscopy.

   Nuclear and electronic spin. Interaction with a magnetic field. Nuclear magnetic resonance (NMR) spectroscopy. Energy levels and selection rules. Nuclear shielding. Chemical shift. Spin-spin coupling. Other MR spectroscopies.

Lab Sessions:

A total of five sessions (4 hours each), plus a sixth session of evaluation (order to be determined). The contents will be:

1. Basic experimental techniques in spectroscopy (I): IR of gas and liquid samples.
2. Basic experimental techniques in spectroscopy (II): UV-VIS and NMR
3. Simulation of Vibrational Spectra
4. Simulation of Electronic Spectra
5. Simulation of NMR Spectra
6. A Project/Case, worked out in the simulation sessions (3 to 5 above).