LU3Ci001: Quantum mechanics and spectroscopies

Persons in charge

P1 and P2

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1. Prospectus

Teaching hours: lectures 24 h, tutorial classes 24 h, preparation to laboratory experiments 2 h, laboratory experiments 10 h

Number of credits: 6 ECTS

Grading /100: in-class exam /70 (integral in-class exam), laboratory /30 (including a practical exam; no restrictions for taking the practical exam)

Paths: mono-disciplinary / bi-disciplinary / top-minor

Period of teaching in English: semester S5 (period P1) of the 3rd-year Bachelor in Chemistry

2. Pedagogic aims of the course

a. Objectives

Know how to:

- relate physical quantities and mathematical tools;
- write the Hamiltonian operator of an atomic or molecular system and the corresponding Schrödinger equation;
- apply an operator onto a wave function, write the normalization condition;
- demonstrate that a function is the eigenfunction of the Hamiltonian operator;
- go beyond the electronic configuration spectral terms;
- associate a type of spectroscopy to a theoretical model (knowledge of the principles of the different studied spectroscopies and interpretation of a spectrum in terms of physical processes)
- validate a theoretical model by comparison between predictions and experimental data.

b. Topics covered

Basis and formalism of quantum mechanics: wave function and probability density, operators and Schrödinger equation;

Applications: particle in a box, energy quantification and quantum number, harmonic oscillator, kinetic momentum (rigid rotor), spin and tunneling effect;

Structure of atoms (atomic orbitals, Slater model and introduction to spectral terms) and of molecules (molecular orbitals and symmetries);

Atomic and molecular spectroscopies (IR, UV-vis and X-ray). Transition momentum. Selection rules. Emission, absorption, scattering. Electronic, vibrational and rotational spectra.

3. Pre-requisites

Chemistry

Atomistic of the LU1Ci001 teaching unit, spectroscopies of the LU2CI005 teaching unit, molecular orbitals and molecular symmetries of the LU2CI001 teaching unit.

Classical physics

Kinetic, potential and total energies, Coulomb force, kinetic momentum and waves.

Mathematics

Usual functions and derivatives, simple and multiple integrals, integration by parts, simple differential equations, matrix.