

# Structures et symétries moléculaires

## Lecturers

Emilie CAUET (Coordinator), Antoine Aerts and Sophie Bauduin

## Course mnemonic

CHIM-F304

## ECTS credits

5 credits

## Language(s) of instruction

French

## Course period

First term

## Campus

Solbosch

## Course content

Electronic structure of atoms (spin and orbital angular momenta, electronic configurations and states, spin-orbit coupling). Molecular structures (Born-Oppenheimer approximation, potential energy surfaces and reactivity). Molecular symmetries and symmetry groups Theory. LCAO theory of molecular orbitals (diatomic and polyatomic molecules, Hückel's theory of conjugated systems, organic molecules and polymers). Nuclear degrees of freedom (separation of motions and energy levels). Molecular rotation (rigid rotor and nonrigid molecules). Molecular vibration (Harmonic oscillator model, normal modes and anharmonicity).

## Objectives (and/or specific learning outcomes)

Build the quantum structure of electronic systems, from the simplest atoms up to complex molecules. Link the theoretical concepts with the other matters and teachings of the Chemistry cursus (organic and inorganic chemistry, biochemistry, polymer and solid state chemistry). Provide the pre-requisites of Master courses (Spectroscopy, kinetics, quantum reactivity, computational chemistry, group theory applications,...)

## Pre-requisites and co-requisites

### Co-requisites courses

CHIM-F206 | Mécaniques classique et quantique | 10 crédits and  
MATH-F214 | Compléments de mathématiques | 5 crédits

## Teaching method and learning activities

Oral teaching ("ex cathedra") using the support slides and black board, interfacing with the Virtual University. Copies of slides and complements provided to the students.

## References, bibliography and recommended reading

- > Mc Quarrie and Simon, "Physical Chemistry, a Molecular Approach", University Science Books (1997). - Atkins and de Paula, "Physical Chemistry", Oxford University Press (2006). - Gill, "Orbitals in Chemistry, Cambridge (2000).

## Course notes

Université virtuelle

## Other information

### Place(s) of teaching

Solbosch

### Contact(s)

Campus Solbosch, Bâtiment D 7e niveau, DC7.222

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## Evaluation method(s)

Oral examination

### Evaluation method(s) (additional information)

Oral examination

### Main language(s) of evaluation

French

## Programmes

Programmes proposing this course at the faculty of Sciences

BA-CHIM | Bachelor in Chemistry | unit 3