



SC

CHIM1180 **Eléments de chimie physique moléculaire**

[45h+22.5h exercises] 5 credits

This course is taught in the 2nd semester

Teacher(s): Daniel Peeters
Language: french
Level: 1st cycle course

Aims

"Elements of molecular physical chemistry" presents some aspects of the atomic and molecular microscopic world to chemists. It aims to describe the electronic structure of atoms and molecules, the geometry of molecules and their internal motions in relation with molecular properties and chemical reactivity. Special attention is paid on the discrete character of energy levels. It introduces the concepts and terminology that will be needed by lectures on molecular spectroscopy, statistical thermodynamics and quantum chemistry.

Main themes

Description of the molecular structure and internal motions
Basic concepts of quantum mechanics (postulates and operators)
The Schroedinger equation and solutions obtained for the hydrogen atom.
Extension to many-electron atoms (Wavefunctions and orbitals; electronic configurations, Pauli principle)
Molecular structure, molecular orbitals, LCAO approximation and related concepts

Content and teaching methods

Starting from a classical description of molecules, the limitations of classical mechanics are presented to introduce quantum mechanics. The Schroedinger equation is presented and solutions are obtained for simple problems (Particle in the box, harmonic vibrator, rigid rotator). Atomic solutions are built for the hydrogen atom and further generalised to many-electron wavefunctions for atoms. Introducing the Born Oppenheimer principle, the molecular structure is described and discussed. Finally the nature of the chemical bond is presented. Various chemical concepts such as symmetry orbitals, hybridisation, sigma-pi separation, Self Consistent Field are introduced.

Other credits in programs

CHIM12	Deuxième candidature en sciences chimiques	(5 credits)	Mandatory
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