

6.00 credits

45.0 h + 22.5 h

Q2

Teacher(s)	Gonze Xavier (compensates Hautier Geoffroy) ;Hautier Geoffroy ;
Language :	French
Place of the course	Louvain-la-Neuve
Main themes	<p>The course focuses on the understanding, using first principles of physics, of the electronic behavior of atoms and molecules and its link to chemistry. It also addresses the understanding of atomic motions in molecules (rotations, vibrations).</p> <p>To do this, the course includes a presentation of the necessary basics of quantum mechanics for the chemist.</p>
Learning outcomes	<p>At the end of this learning unit, the student is able to :</p> <p>The course, intended for chemistry students, gives an introduction to the microscopic aspects of the atomic and molecular world.</p> <p>It introduces concepts such as the electronic structure of atoms and molecules, the geometrical structure of molecules as well as the molecular movements, with the idea of relating these concepts to molecular properties and chemical reactivity.</p> <p>¹ Special attention will be given to the discrete character of energy levels, to their significance, to the way they are calculated as well as to the description of individual molecules.</p> <p>The course serves as an introduction to molecular spectroscopy, to statistical thermodynamics and to quantum chemistry.</p> <p>It introduces terminology and concepts needed in organic and inorganic chemistry.</p>
Evaluation methods	Students will be evaluated by a written exam without access to support.
Teaching methods	Ex cathedra lectures, visualisation of videos and optional question/answer sessions, and exercise sessions.
Content	<ul style="list-style-type: none"> - Elements of quantum mechanics : History, foundations, basic concepts, postulates and operators in quantum mechanics, resolution of simple systems. Schrodinger equation. - Hydrogen atom. - Approximate methods (variation theorem and perturbative approaches). - He atoms and other multi-electronic atoms. Notion of spin, indistinguishability and anti-symmetry. - Hartree-Fock equations. - Born-Oppenheimer approximation. Diatomic and polyatomic molecules. Theory of molecular orbitals. - Quantum approach of vibrations and rotations in diatomic and polyatomic molecules. - Interaction of light with molecules and atoms. Selection rules.
Inline resources	moodle site : https://MOODLE.UCLOUVAIN.BE
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Bachelor in Chemistry	CHIM1BA	6		