UCLouvain

lchm1252

2020

Elements of physical molecular chemistry

Due to the COVID-19 crisis, the information below is subject to change, in particular that concerning the teaching mode (presential, distance or in a comodal or hybrid format).

6 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
Aims	1 The course, intended for chemistry students, gives an introduction to the microscopic aspects of the atomic and molecular world. 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. 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. The course serves as an introduction to molecular spectroscopy, to statistical thermodynamics and to quantum chemistry. It introduces terminology and concepts needed in organic and inorganic chemistry. - - - - *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Evaluation methods	**Due to the COVID-19 crisis, the information in this section is particularly likely to change.** Students will be evaluated by an open book written exam. Due to the COVID-19 crisis, the evaluation may be done by distance.
Teaching methods	**Due to the COVID-19 crisis, the information in this section is particularly likely to change.** Ex cathedra lectures and exercice sessions. Due to the limited capacity of auditoria this year (COVID-19 crisis), some classes or exercices could be given remotey or co-modally.
Content	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.
Faculty or entity in charge	CHIM

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