UCL Université catholique de Louvain

LCHM1252

2015-2016

Elements of physical molecular chemistry

6.0 credits	45.0 h + 22.5 h	2q

Teacher(s) :	Hautier Geoffroy ;
Language :	Français
Place of the course	Louvain-la-Neuve
Prerequisites :	*The prerequisite(s) for this Teaching Unit (Unité d'enseignement – UE) for the programmes/courses that offer this Teaching Unit are specified at the end of this sheet.*
Main themes :	- Molecular structure and description of internal movements. Starting from lagrangian analytical mechanics, molecular internal coordinates are introduced, normal modes deduced and molecular vibrations obtained. A brief introduction to molecular mechanics, to force fields and their applications in chemistry, including conformational analysis, is given. - Elements of quantum mechanics: Fundamentals, basic concepts, postulates and operators in quantum mechanics are proposed completed by the resolution of simple systems. - Physical molecular theoretical chemistry : Application of Schrödinger equation to polyelectronic systems : Spin and antisymmetry ; Introduction to shell models; Orbital approximation and the Hartree-Fock model; Atomic orbitals, electronic configurations, multiplicity and atomic terms are discussed. Molecular orbitals, LCAO-MO method, Molecular Structure and hybrid orbitals are presented. - Introduction to quantum chemistry, its methods and their terminology : Hoffmann methods, Huckel, xxDO, ab Initio, etc. ; chemical properties: ionisation potential, electronic affinity, electro negativity, resonance energy. Frontier orbitals and their applications, symmetry conservation and chemical reactivity ; geometry and electronic structure of molecules, ions and radicals.
Aims :	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".*
Other infos :	Exercises focus on the molecular aspects, more particularly on rotational and vibrational movements, molecular mechanics, description of simple chemical components, pi systems and frontier orbitals. They are aiming to illustrate the different theoretical concepts and put them into practice. The use of current software allowing molecular representation is required. A tight coordination with the course of crystallography and molecular spectroscopy is necessary.
Faculty or entity in charge:	CHIM

Programmes / formations proposant cette unité d'enseignement (UE)

Intitulé du programme	Sigle	Credits	Prerequis	Acquis d'apprentissage
Bachelor in Chemistry	CHIM1BA	6	LMAT1111F **and** LMAT1111G **and** LPHY1121 **and** LPHY1122	