UCL Université catholique de Louvain

LBIR1314

2013-2014

Physical chemistry I

4.0 credits	30.0 h + 22.5 h	2q

Teacher(s) :	Gaigneaux Eric (coordinator) ; Gonze Xavier ;
Language :	Français
Place of the course	Louvain-la-Neuve
Inline resources:	Icampus
Prerequisites :	LBIR1200 Mathématiques générales II (or équivalent course) LBIR1210 Physique générale (II) (or équivalent course)
Main themes :	Quantum mechanics of atoms and molecules : introduction to the formalism of quantum mechanics, structure of atoms and molecules, nature of chemical bond. Spectroscopy : principles of the different major spectroscopies for chemistry.
Aims :	a. Contribution de l'activité au référentiel AA (AA du programme) LBIR1314 contributes to the learning outcomes B1.3, B1.5, B3.5 et B3.6. b. Formulation spécifique pour cette activité des AA du programme (maximum 10) At the end of the activity, the student is able of : - stating and explaining the concepts at the basis of quantum mechanics, demonstrating the fundaments of some mathematical relationships thereof, and applying these concepts to atoms and biatomic molecules ; - stating and explaining the fundamental characteristics of the eigenvalue and eigenfunctions of the Schrödinger equation, for a series of simple potentials, and to separate variables to analyze the case with several variables; - explaining the constitution of the periodic table of the elements and, starting from atomic orbitals, explaining the formation of molecular orbitals and of the chemical bond in biatomic molecules ; - solving simple problems related to the calculation of average values of operators, of probability densities, of absorption and emission spectra, of formation energy, and of excited states (electronic, vibrational, rotational) of atomic and molecular systems; - distinguishing between absorption and emission spectrocopies ; - assigning the spectrum of a given compound to the corresponding spectroscopic technique from which it is obtained, and extracting the useful information from the said spectrum; - predicting the main characteristics (number of peaks, distance between peaks, energy range, etc) of the rotation, vibration, Raman, XPS, EPR, NMR spectra expected for a given sample, and when it applied predicting the impact (peak shift) when the said sample undergoes an isotopic shift; - correlating the difference in peaks position between two samples and their respective characteristics, such as length of a chemical bond (rotation spectroscopy), bon strenght (IR and Raman), nature of the bond (UV-Vis), oxidation states of the elements (XPS), etc. *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 :	During a written examination, several theory questions and problems are proposed to the students. The students demonstrate their knowledge by stating and explaining the related content of the lectures, and demonstrate their ability to solve these problems by actually solving them and explaining their methodology. For the spectroscopy part more specifically, quantitative problems are proposed, aiming the exploitation of spectra features in order to calculate the characteristics of the samples from which they are obtained (and vice versa : predicting the spectra of samples with known characteristics).
Teaching methods :	Ex cathedra lessons and exercice sessions.
Content :	Introduction to quantum mechanics (20h): Schrödinger equation and its solutions for a particlein a potentiel well (box, harmonic oscillator, rigid rotator, hydrogenoid atoms). Generalisation towards polyelectronic atoms, the molecular ion H2+, the hydrogen molecule and diatomic molecules by describing the molecular motion and the concept of chemical bond. Fundaments of spectroscopy (10h) : distinctions between spectrocopy et spectrometry, between absorption and emission spectroscopies, fundaments of rotation, vibration, libration, rotation and vibration Raman, UV-Vis, XPS, RPE and RMN spectroscopies. Spectroscopy (7.5 h) : distinctions between spectroscopy and spectrometry, emission and absorption, rotational, vibrational and libration spectroscopies with special emphasis on the principles, differences and complementarity of IR and Raman vibrational spectroscopies, electron spectroscopy with special attention on the difference between UV-Vis spectroscopy and photoelectron spectroscopy, principles of resonance spectroscopies (ESR and RMN). Exercices are organized with the objectives to acquire the ability to distinguish and handle spectra from different spectroscopies and to retrieve information from them related to the analyse samples.
Bibliography :	No compulsory books, some of them being however recommended.

Other infos :	
Cycle and year of study :	> Bachelor in Bioengineering
Faculty or entity in charge:	AGRO