UCLouvain

lchm1252

2023

Elements of physical molecular chemistry

6.00 credits	45.0 h + 22.5 h	Q2

Teacher(s)	de Wergifosse Marc ;
Language :	French
Place of the course	Louvain-la-Neuve
Main themes	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). To do this, the course includes a presentation of the necessary basics of quantum mechanics for the chemist.
Learning outcomes	**At the end of this learning unit, the student is able to :** 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.
Evaluation methods	Exercise questions account for 15% of the final score. The laboratory report accounts for 5% of the final grade. Students will be assessed by a two-part examination (80% of the final grade): closed-book written and oral.
Teaching methods	Interactive lectures with optional Q&A sessions. Compulsory exercise sessions and a compulsory laboratory are organized to facilitate student comprehension. With the exception of the first session, each exercise session includes a short 15-minute quiz on the previous session's material. A report will be requested for the laboratory session.
Content	**Chapter 0: Mathematics reminder** 1. Complex numbers 2. Vectors and matrices 3. Differential equations **Chapter 1: The origins of quantum mechanics** 1. Introduction 2. Origins of quantum mechanics 3. Black-body radiation 4. The photoelectric effect 5. The Compton effect 6. The atomic spectrum of hydrogen 7. Bohr's model 8. Wave/corpuscle duality **Chapter 2: The foundations of quantum mechanics** 1. Operators in quantum mechanics 2. The postulates of quantum mechanics 3. Characteristics and evolution of states **Chapter 3: Linear motion** 1. Characteristics of wave functions 2. General remarks on Schrödinger's equation 3. Linear translational motion • A free particle in a one-dimensional system • Penetration through a potential energy barrier • A particle in a box

	1. Linear motion • The harmonic oscillator • The harmonic oscillator for a diatomic molecule **Chapter 4: Rotations** 1. Rotation of a particle on a circle 2. Rotation of a particle on a sphere 3. The rigid rotator as a model for the rotation of a diatomic molecule 4. Angular momentum **Chapter 5: The hydrogen atom** 1. Movement of an electron in a Coulomb potential 2. Single-electron atomic orbitals 3. Back to angular momentum **Chapter 6: Approximation techniques** 1. Time-independent perturbation theory 2. Method of variations **Chapter 7: The helium atom and spin** 1. The Helium atom 2. Spin 3. Spin and Helium 4. Hartree product 5. Slater determinants **Chapter 8: Polyelectronic atoms and the Hartree-Fock method** 1. Polyelectronic atoms 2. Slater atomic orbitals 3. Hartree-Fock method 4. Time-dependent perturbation theory 5. Atomic spectra 6. Spectroscopic notation of an electronic configuration 7. Hund's rules for determining the atomic term of the ground state 8. Selection rules for polyelectronic atoms **Chapter 9: Introduction to molecular structure** 1. The Born-Oppenheimer approximation 2. The H2+ ion 3. Molecular orbital theory 4. The dihydrogen molecule 5. Diatomic molecules 6. The electronic term for an electronic state of a diatomic molecule 7. Excited states of diatomic molecules 8. Molecular orbital theory for polyatomic molecules 9. Why is the BeH2 molecule linear and the H2O molecule angled? 10. A few words on Hückel's method **Chapter 10: Interaction of molecules with light** 1. Reminder: Time-dependent perturbation theory 2. Selection rules for absorption and emission 3. Electronic spectroscopy 4. Vibrational spectroscopy of diatomic molecules 5. Vibrational spectroscopy of polyatomic molecules
Inline resources	moodle site : https://MOODLE.UCLOUVAIN.BE
Other infos	Understanding this teaching unit requires weekly work on the part of the student, as the concepts are built up as the course progresses. Attendance is therefore strongly recommended.
Faculty or entity in charge	CHIM

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