UCLouvain

lbirc2105

2022

Physical chemistry II

5.00 credits	45.0 h + 15.0 h	Q1

Teacher(s)	Debaste Frédéric (coordinator) ;Debecker Damien ;Supiot Philippe (compensates Debecker Damien) ;
Language :	French > English-friendly
Place of the course	Louvain-la-Neuve
Main themes	Implementation of two complementary physico-chemical approaches for the forecast and the command of properties of matter Macroscopic properties and molecular interpretation - Kinetics: Knowledge of fundamental laws regulating the progress of chemical reactions// Interpretation of kinetics experimental data to deduce reaction mechanisms. - Phase equilibria: Study of phase equilibria of condensed systems (liquid/liquid; liquid/solid) and of liquid/vapor systems with several constituents: interpretation and use of phase equilibrium diagrams // Thermodynamic study of nonideal systems with several constituents (solutions): use of thermodynamic tools for solving phase equilibrium problems. Properties of particles and forecast of macroscopic properties - Statistical mechanics. Basic concepts // Application to gaseous systems // a priori calculations of thermodynamic quantities // Application to chemical free energy // Notions of non-equilibrium thermodynamics.
Learning outcomes	**At the end of this learning unit, the student is able to :** 1 Knowledge concerning the properties of matter and their understanding from the corpuscular/molecular scale. Know-how in physical chemistry: quantification, conceptualisation, modelling. Development of an adequate attitude towards the understanding of the properties of matter and their command.
Evaluation methods	Written exam, covering all the learning outcomes (both theory and exercices).
Teaching methods	Ex cathedra course, with powerpoint slides as a visual support. The slides are provided via Moodle in the beginning of the semester. They are only a support and do not contain all the needed information. Context, examples, motivation, exercices, visual representation, mathematical developments are presented orally and on the blackboard during the course. Exercices sessions are oganized (7 sessions).
Content	**Introduction**: context and objectives. Particalities. Information about the exam. **Part 1: KINETICS** Rate of chemical reaction. Relationship with chemical thermodynamics. Rate equations of chemical processes. Activation energy. Reaction orders. Influence of temperature. Absolute reaction rates theory. Collision and transition state theory. Irreversible and reversible reactions. Parallel and consecutive reactions. Degeneration of orders. Catalytic reactions kinetics. Kinetics of polymer formation reactions. Chain reactions. **Part 2: PHASE EQUILIBRIUM** Binary liquid-liquid, liquid-solid and liquid-vapor phase diagrams, ternary diagrams. Thermodynamics of nonideal and ideal solutions. Use of thermodynamic tools for the study of colligative properties of the diluted solutions (vapor pressure, boiling point, freezing point and osmotic pressure). **Part 3: STATISTICAL MECHANICS** Introduction and fundamental concepts. Definition of ergodicity, microstate, configuration. Kinetic theory and the equation of state of a gas. Botlzmann law and partition functions. A priori calculation of thermodynamic quantities. Application to chemical equilibrium. Introduction to non-equilibrium thermodynamics. Methods Courses and exercises concentrating on concrete use of the concepts.
Inline resources	Moodle: - slides are posted in advance. Students are encouraged to bring them to the course to annotate the slides. - exel files allowing to visualize some of the concept explained in the course, in the fom of plots. - recap of important formula and retranscription of some of the mathematical developments. - list of exercices covered during the practical sessions.
Bibliography	Aucun support payant n'est obligatoire. Une impression des diapositives (powerpoint) utilisées au cours et préalablement mises à disposition sur Moodle est vivement recommandée. Comme supports de cours facultatifs et disponibles en bibliothèque : - D.A. Mc Quarrie, J.D. Simon, Physical Chemistry. A molecular approach, University Science Books, 1997 - Atkins & De Paula, Chimie Physique, Ed. De Boeck Université, 2008

Other infos	This course can be given in English.
Faculty or entity in charge	AGRO

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Master [120] in Chemistry and Bioindustries	BIRC2M	5		