

8.00 credits

45.0 h + 60.0 h

Q2

Teacher(s)	Devillers Michel ;Hautier Geoffroy ;Leyskens Tom (compensates Hautier Geoffroy) ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	<i>The prerequisite(s) for this Teaching Unit (TU) are specified at the end of this sheet, in relation to the programs/ training courses that offer this TU.</i> <i>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.</i>
Main themes	<b>0. INTRODUCTION TO PHYSICAL CHEMISTRY.</b> Chemical equilibrium and partition coefficients. Applications. <b>1. THERMODYNAMICS.</b> First principle of thermodynamics. Thermochemistry. Second principle of thermodynamics. Free Enthalpy. <b>2. PHASE EQUILIBRIA.</b> Generalities. One-component systems: state diagram of a pure body. Thermodynamics and phase transition temperature. Phase rule. Two-component systems: binary phase diagrams. <b>3. CHEMICAL EQUILIBRIA IN SOLUTION.</b> Solubility and complexation. Complex reaction networks. Quantitative study of some cases. <b>4. COMPLEMENTS OF ELECTROCHEMISTRY.</b> Electrolysis. Conductivity of solutions. Batteries.
Aims	Quantitative interpretation of chemical phenomena based on physicochemical laws. Introduction to the use of data tables. <sup>1</sup> <i>The contribution of this course to the development and mastery of the skills and knowledge of the program(s) is available at the end of this sheet, in the section "Programs/training courses offering this course".</i> ----- <i>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".</i>
Evaluation methods	<b>Due to the COVID-19 crisis, the information in this section is particularly likely to change.</b> Written exam at the end of the year, supplemented by continuous assessment during the year (preparation of lab sessions and reports). This part of the grade from the continuous assessment will be used for each session and may not be repeated. <b>Practical training</b> is an integral and inseparable part of the general chemistry course. Participation in all practical sessions is therefore <b>MANDATORY</b> . The laboratories are taken into account in the final grade of LCHM1211 taken into account in the deliberation. Any <b>REASONED</b> absence (justified by a medical certificate in case of illness, or by an official document in other cases) will result in the recovery of the missed session during the last week of the term. Any <b>NON-MOTIVATED</b> absence will in principle be sanctioned by a <b>NEGATIVE mark of 5 POINTS</b> on the final mark of LCHM1211 taken into account in the deliberation, and may, depending on the degree of recurrence and the assessment of the situation by the teaching staff, result in a <b>non-negotiable final mark of ZERO out of 20</b> . Should the number of unjustified and/or justified absences become significant, the teaching staff reserves the right to activate the articles of the RGEE allowing the jury to prohibit the student from registering for the corresponding exam.
Content	<b>I. Thermodynamics</b> First principle of thermodynamics 1. Internal energy, work, heat. Conservation of total energy, first principle. Enthalpy. Molar heat. Global enthalpy balance with phase changes. Adiabatic transformation and calorimetry. Applications of the 1st principle to chemical transformations: Thermochemistry 2. Thermochemical equations: with heat balance. H and U are state functions. Hess's law. Standard enthalpy of formation. Standard enthalpy of combustion. Enthalpy of atomization. Enthalpy of binding. Standard enthalpy of reaction. Thermochemistry of solutions. (DH <sup>f°</sup> ) of ions in aqueous solution. Applications and illustrations of the concepts (e.g. acid-base neutralization). Variation of DH with temperature. The second principle of thermodynamics.

3. Entropy and disorder. Spontaneity. Standard entropy as a function of temperature. Standard entropy of reaction. Microscopic interpretation of entropy. Global variation of entropy. Free enthalpy.  
 4. Definition. Relation with spontaneity. Standard free enthalpy of formation. Standard free enthalpy of reaction. Influence of temperature on spontaneity. Non-spontaneous reaction becoming spontaneous at another temperature.  
 Applications and illustrations (e.g. Ellingham diagrams for the reduction of oxides). Chemical equilibrium and thermodynamics  
 5. Entropy of mixing. Link with the equilibrium constant. Reaction of equilibria to changing conditions.  
 Van't Hoff relation: influence of T on K.

## II. Phase equilibria

Generalities

1. Definitions: physical states of matter, phase, constituents. One-component systems: state diagram of a pure body  
 2. P-T diagrams of a one-component system. Link between thermodynamics and one-component phase diagrams. Gibbs' phase rule. Examples of one-component P-T diagrams (H<sub>2</sub>O, CO<sub>2</sub>, Fe, ..). Multi-component systems  
 3. Phase diagram of multicomponent phases. Link between thermodynamics and multicomponent phase diagrams. Entropy of mixing and free enthalpy for ideal solutions. Multi-component phase rule. Construction of phase diagrams from free enthalpy curves: common tangent rule. Reading phase diagrams: lever rule. Colligative properties of solutions  
 4. Cryoscopy, ebullioscopy. Entropy of mixing and free enthalpy for regular solutions. Applications and illustrations with binary phase diagrams (liquid-gas, liquid-solid, solid-solid).

## III. Chemical equilibria in solution

A/ Complements of acid-base equilibria and pH-metry: Mixtures of several solutes. Polyfunctional solutes.

B/ Complex reaction networks: Reminders on acid-base, solubility and complexation chemical equilibria. Reactions of an acid with a weakly soluble acid salt. Precipitation of a weak acid salt. Precipitation of a hydroxide in the presence of a weak base. Competition between precipitation and complexation. Quantitative study of some cases: Selective precipitation of sulfides, Solubilization by complexation.

## IV. Complements of electrochemistry

Reminder on electrochemical cells: electrolysis and batteries. Notions of electricity. Electrolysis

1. General principle. Faraday's laws. Reactions at electrodes and industrial applications. Conductivity of solutions  
 2. Principles and definitions. Mobility of ions. Experimental aspects. Transport numbers and balance of an electrolysis. Applications: Degree of dissociation of a weak electrolyte. Ionic product of water. Determination of a solubility product. Conductimetric titrations. Batteries, or galvanic cells  
 3. Reminders: electromotive force of a battery, standard electrode potential and Nernst relation, energy balance of the battery. Main types of electrodes: metal-ion electrodes, insoluble metal-salt electrodes, gas electrodes, redox electrodes. Analytical applications: pH measurement, potentiometric titrations, commercial batteries, primary batteries, secondary batteries, or accumulators, fuel cells.

### Laboratory sessions (4x3h + 4x3h30) :

Each student individually prepares and performs an experiment illustrating a theme of the course. They write a report. A laboratory manual allows the student to prepare each laboratory session. A verification of this preparation takes place at the beginning of each session.


### Exercise sessions (13 x 2h) :

Solving theoretical problems and numerical exercises in the presence of assistants.

**Part LCHM1211A and LCHM1211B do not include part A of chapter III. It includes only 4 laboratory sessions of 3 hours and 7 exercise sessions of 2 hours.**

Supervision: weekly individualized contacts in order to answer specific questions.

Inline resources	moodleucl
Bibliography	Livre de P. Atkins, L. Jones et L. Laverman : "Principes de Chimie", Trad. Française de A. Pousse (De Boeck), ou édition anglaise originale correspondante, complété par des notes de cours. Manuel de travaux pratiques et fascicule d'exercices. Documents fournis sur Moodle.
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Aims
Bachelor in Chemistry	CHIM1BA	8	LCHM1111 AND LPHY1101 AND LPHY1102	
Minor in Chemistry	MINCHIM	8		