# CHIMIE PARISTECH - PSL

## Syllabus

## 1st year of the engineering cycle


Chimie Paris
ParisTech
PSL

The first year is dedicated to the training of multidisciplinary general science, to provide the student engineer with a complete level of scientific knowledge.

Teaching includes basic courses in mathematics, physics, computer science, courses oriented towards the theoretical foundations of chemistry (physicochemistry, structure of matter) and courses in organic and analytical chemistry. The courses are supplemented by one-day experimental works designed to teach the basic gestures of chemistry, starting with safety rules and risk management.

The engineering professions are introduced through management courses focused on the discovery of the business world and in the second semester, over a period of six months, a transdisciplinary project allowing students to learn to manage teamwork while being able to report to a client. At the end of the year, after the last exams which take place at the beginning of May, the students manage a three-week project in research laboratories.

The school year terminates with a one or two-months internship

| **Semester 1:** | **Semester 2:** |
|---|---|
| **Mathematics and physics for the engineer (6 ECTS)**<br>Applied mathematics for engineers<br>Quantum Mechanics<br>Computer science and programming<br><br>**Physical and analytical chemistry (6 ECTS)**<br>Physico-chemistry of interfaces<br>Experiments in Physical and analytical chemistry<br><br>**Molecular chemistry 1 (6 ECTS)**<br>Structure and reactivity<br>Molecular Spectroscopy<br>Chemical risk<br><br>**Structure of the material (6 ECTS)**<br>Solid chemistry<br>Crystallography<br><br>**Business knowledge, languages and culture 1 (6 ECTS)**<br>Management<br>English<br><br>**Optional courses**<br>Sport<br>Foreign language | **Material and interactions (6 ECTS)**<br>Chemical bonding<br>Matter-Radiation Interaction<br>Experiments in Spectroscopy<br><br>**Molecular chemistry 2 (6 ECTS)**<br>Synthesis and reactivity<br>Long experimental projects<br>Experiments in molecular chemistry<br><br>**Processes (6 ECTS)**<br>Chemical engineering<br>Numerical methods<br>Experiments in chemical engineering<br><br>**Analytical chemistry (6 ECTS)**<br>Solution chemistry<br>Separation methods<br>Electrochemistry<br>Experiments in Physical and analytical<br><br>**Business knowledge, languages and culture 2 (6 ECTS)**<br>Management<br>English<br>Transdisciplinary project<br>Worker internship<br><br>**Optional courses**<br>Sport<br>Foreign language |

# SEMESTER 1

| 1A S1 | MH11ES.MAI | **Applied mathematics for engineer**<br>*Key words :* algebra, Fourier transform, statistics |
|---|---|---|

Responsible : Frédéric Wiame Maître de conférences
frederic.wiame@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Written exam |
|---|---|---|---|---|---|
| | 0 h | 24 h | 0 h | | |

***Course outline :***

Chimie Paris mathematics course provides students with the essential notions of mathematics allowing them to understand first-year courses and practical work (Physics I: Quantum Mechanics, Physics II: radiation-matter interactions, TP IRM and Materials ...). It is thus a teaching with applied purpose for which practicing of concepts is essential.

The course is divided into three parts:

1) Mathematics applied to quantum mechanics where are introduced the notion of Hilbert space, the Dirac notation, the computation of quantities in a complex vector space, and their application in the framework of the theory of measurement in quantum mechanics.

2) Mathematics applied to signal processing where are discussed the use of Fourier series and Fourier transforms as tools for processing and analysis.

3) Mathematics applied to data analysis where are presented the notions of probabilities, statistics and distributions. Essential concepts such as mean, standard deviation, and linear regression will be reported and applied to error calculations and data analysis.

***Learning objectives :***

At the end of the course students will be able:

- to use Dirac's formalism and computation in a Hilbert space in the context of a quantum physics or quantum chemistry problem,
- to analyze a signal and to understand a process for processing or producing a signal by using the properties of Fourier transformation and Dirac distribution,
- to assess uncertainties about a measured quantity in a relevant way and to understand the principles underlying data analysis methods.

***Prerequisites :***

***Teaching language :*** french

***Documents, website :*** handouts, slide presentation, online quiz https://coursenligne.chimie-paristech.fr/course/view.php?id=29

| 1A<br>S1 | MH11ES.MQ | **Physics I : Quantum Mechanics**<br>*Key words :* fundamental concepts of quantum physics, model systems |
|---|---|---|

Responsible : Laurent Binet, Maître de Conférences, Chimie ParisTech
laurent.binet@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* written examination |
|---|---|---|---|---|---|
| | 12 h | 12 h | 0 h | | |

***Course outline :***

This course aims at introducing the conceptual tools necessary to address future technological innovations (e.g. quantum technologies) in which chemistry is to play a key role, to understand the functional properties of molecules and materials and to appropriate the advanced methods for the characterization of matter. The course thus introduces the postulates of quantum mechanics, the mathematical tools, the main model systems (potential wells and steps, the harmonic oscillator, the hydrogen atom), the angular momenta and the importance of symmetry in physics.

***Learning objectives :***

The student should be able to:

- Tell the conceptual differences between classical and quantum physics.
- Use the mathematical formalism of quantum mechanics.
- Apply the postulates in the context of a measurement problem.
- Define the main features and properties of the model systems.
- Use appropriate approximations to change a complex system into a model system.

***Prerequisites :***

Undergraduate knowledge in classic mechanics and mathematics as taught in Bsc of physics

***Teaching language :*** french (english on request)
***Documents, website :*** https://coursenligne.chimie-paristech.fr

| 1A<br>S1 | MH11ES.IP | **Computer science and programming**<br>*Key words :* programming, C |
|---|---|---|

Responsible : Frédéric Labat Maître de Conférences
frederic.labat@chimie-paristech.fr

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Computer-based evaluation |
|---|---|---|---|---|---|
| | 0 h | 26 h | 0 h | | |

***Course outline :***
This module aims to train the engineering student in the basic concepts of programming, and to enable him/her to build an application independently using simple and familiar algorithms.
The programming language used is C, which is fundamental in industrial and academic fields. This makes it possible to introduce fundamental aspects of programming such as the choice of appropriate representations of data in memory, notions of numerical precision, the proper use of the results of numerical calculations or the structure or logic of a program when building an application to solve a given problem.
Particular attention is paid to the efficiency, quality and limitations of IT solutions, in order to make the student engineer able to communicate with the IT specialists of his future company or laboratory, and to remove the black box aspect generally associated with IT.
The training is based on course/TD sessions, based on examples mainly taken in the field of chemistry using the free software Code::Blocks, easily installed on any personal computer.

***Learning objectives :***
The student must be able to:
- analyse a problem and translate it into a general programming language
- imagine and design an application using a modular structure and an appropriate representation of the data in memory
- evaluate, control and validate algorithms and programs

***Prerequisites :***
None

***Teaching language :*** french
***Documents, website :*** handouts, documents

| 1A<br>S1 | MH11ES.PCI | **PHYSICO-CHEMISTRY AND INTERFACES**<br>*Key words :* mixing, ideality, non-ideality of physico-chemical systems, interfaces and colloids |
|---|---|---|

Responsible : Virginie LAIR
virginie.lair@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Final written exam |
|---|---|---|---|---|---|
| | 12 h | 12 h | 0 h | | |

***Course outline :***
The first part of the PCI course focuses on the concepts necessary to study chemical equilibria with emphasis on the notion of chemical potential and intensive molar quantities particularly derived from thermodynamics (enthalpy, free enthalpy and entropy).
We will use thermodynamics to relate a priori independent properties and express the effects of variables such as temperature and pressure. We will apply these notions to gases, ionic solutions and binary mixtures (liquid/gas), insisting on the notion of ideality and non-ideality. We will see how to develop valid models for real behaviors (van der Waals, Debye-Huckel models, regular solutions for example). The notion of activity and activity coefficients will be at the heart of this part while relying on concrete applications of measurements and determination. The colligative properties will also be discussed.
Then, we will introduce the thermodynamic phenomena at the level of liquid surfaces by developing the concepts of surface tension, capillarity, contact angle and adsorption. The thermodynamic and kinetic basis of colloid stability will also be presented.

***Learning objectives :***
To give the future engineer a basic skill, complementary to his training in physical chemistry, on the acquired bases of thermodynamics. The future engineer will be able to :
- Understand and know how to describe a real system according to the basics of the ideal system, gas or solution.
- Understand and assimilate the phenomena at interfaces.
- Acquire the notion of metastability (e.g. emulsions and colloids).

***Prerequisites :*** Basics of thermodynamics, chemical equilibrium, solution chemistry

***Teaching language :*** french
***Documents, website :*** pdf documents, handouts https://coursenligne.chimie-paristech.fr/enrol/index.php?id=8

| 1A<br>S1S2 | MH11FECP et<br>MH12FECP | **Laboratory course in physical and analytical chemistry**<br>*Key words :* physical and analytical chemistry, electrochemistry, chromatography and separation sciences |
|---|---|---|

Responsible : d'Orlyé Maître de conférences
fanny.dorlye@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Practical examination, bibliographic report, experimental reports, oral presentations, daily involvement |
|---|---|---|---|---|---|
| | 0 h | 0 h | 67.5 h | | |

***Course outline :***
The practical work in this module is in harmony with the courses of physical chemistry and interfaces, chemistry of reaction media, electrochemistry and separative methods. They allow to illustrate and to put into practice the theoretical notions of the course as well as to apprehend their fields of application in the industry. The first part of the course concerns the analysis of traces / ultratraces in relation to the fields of quality control, industrial process control and environmental protection: liquid/liquid extraction methods for metal cations (downstream of the nuclear cycle); separative methods (ion chromatography, high-performance liquid chromatography, capillary electrophoresis) for the determination and quantification of inorganic or organic pollutants; electrochemical methods (complexation or pulse polarography, selective electrodes) for the determination and quantification of pollutants in environmental matrices (water, soil) as well as for decontamination (ultrafiltration). A second component concerns studies at interfaces to better understand the synthesis and characterization of new materials and processes using interfaces: synthesis of materials by electrochemical way (electrodeposition); study of corrosion and additives allowing to control this phenomenon; electrokinetic characterization of membranes and application to electrodialysis (water purification); thermodynamics of surfaces (surface tension, contact angle) for the characterization of a formulation of detergents and functionalized surfaces (design of windshields, for example) ; characterization of complex media (hydrogen electrode, densimeter, UV-visible spectroscopy, cyclic voltammetry) for the understanding and prediction of phenomena in industrial processes involving hydro-organic and micellar media, catalytic processes. ..

***Learning objectives :***
Following this practical training, students should be able to:
- Follow health and safety guidelines
- Get pratical laboratory skills
- Fill out a laboratory workbook
- Analyse, exploit and discuss experimental data
- Use appropriate theoretical concepts and models
- Undertake a literature search
- Write experimental and bibliographic reports
- Present experimental results and conlusion to an audience

***Prerequisites :***
thermodynamics of solutions and interfaces

***Teaching language :*** french
***Documents, website :*** handouts, self evaluation quiz, tutorials

| 1A<br>S1 | MH11ES.SR | **Functional Groups: Synthesis and Reactivity**<br>*Key words :* |
|---|---|---|

Responsible : Sylvain Darses
sylvain.darses@chimie-paristech.fr

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Written exam |
|---|---|---|---|---|---|
| | 12 h | 12 h | 0 h | | |

***Course outline :***
The course MH11ES.SR "Functional groups: synthesis and reactivity" addresses the chemistry of carbon compounds through the study of the characteristic reactions of the main functional groups. In this first part of a teaching given over two semesters, the formation and reactivity of the carbon-carbon bonds will be mainly tackled: chemical bonding, hybridization, halogenated derivatives (substitution, elimination, ...), alkenes and alkynes (addition, oxidation, ...), dienes ([4+2]-cyclo-addition, ...), aromatics (electrophilic substitution, reduction, reactivity at the benzyl position, …), alcohols (activation, protection, oxidation, etc.) , amines (formation, protection).

***Learning objectives :***
At the end of the MH11ES.SR module, the students will have acquired some essential basics in organic chemistry and will be able to apprehend the realization of simple synthesis. They will be in possession of the necessary tools to understand and analyze the mechanisms and the reactivity of the molecules, allowing them to deepen their knowledge with the MH12ER.SR module.

***Prerequisites :***
Basic knowledge of organic chemistry

***Teaching language :*** french
***Documents, website :*** handouts

| 1A<br>S1 | MH11ES.SCM | **BASIC PRINCIPLES OF MOLECULAR SPECTROSCOPY**<br>*Key words :* NMR, mass spectrosmetry, molecular spectroscopy, UV-vis, IR, Nuclear magnetic resonance |
|---|---|---|

Responsible : Frédéric de Montigny Maître de Conférences
frederic.de-montigny@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* written exam |
|---|---|---|---|---|---|
| | 9 h | 6 h | 0 h | | |

***Course outline :***

The objective of the course is to present the usual analysis methods for organic molecules. The student should understand the fundamental bases of these methods and should be able to analyze different kinds of molecules. It is divided into three parts: NMR, mass spectrometry and molecular spectroscopy.

* Nuclear magnetic resonance spectroscopy:

- Analysis of 1H and 13C NMR spectra, determination of the covalent structure of organic molecules, NMR principles: spin concept, Zeeman effect, chemical shift, scalar coupling, spectrum recording techniques: 1H NMR: diastereoisotopy, 1st order and 2nd order spectra, … NMR 13C: 1D experiments, uncoupling, ...

* Mass spectrometry:

- The basic principles of mass spectrometry and the characteristics of this spectrometry method (Molecular mass, average, isotopy, resolution, etc.)
- The different ionizations strategies and mass analyzers and their application in the study of more complex compounds.
- General fragmentation rules allowing the analysis of spectra of various organic compounds presenting the main functions encountered in organic chemistry.

* Molecular spectroscopy:

- Reminder of the fundamentals governing IR, UV-vis with a short introduction on Raman, and optical activity....

***Learning objectives :***

Acquisition of theoretical and practical knowledge of mass spectrometry (MS)and Nuclear Magnetic Resonance (NMR). In these lectures, the basic concepts of MS, spectroscopy and NMR are used to understand the applications of these two techniques to identify organic compounds. Exercise sessions will be used to become familiar with interpreting spectra of small molecules and macromolecules.

***Prerequisites :***

***Teaching language :*** french

***Documents, website :*** https://coursenligne.chimie-paristech.fr/enrol/index.php?id=16

| 1A<br>S1 | MH11ES.RC | **Chemical safety**<br>*Key words :* safety, risk assessment, material safety data sheet, fires and explosion, industrial hygienes |
|---|---|---|

Responsible : Michael Tatoulian Professeur
michael.tatoulian@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* written exam |
|---|---|---|---|---|---|
| | 16 h | h | h | | |

***Course outline :***
This course aims first of all to provide the basic elements of chemical risks in order to know how to decipher a safety data sheet and to know all the parameters of toxicological and fire risk assessment. Particular attention will be paid to the physico-chemical properties (SDS) useful for understanding chemical risks. Different exposure scenarios will be presented to allow students to assess the chemical risks related to possible overexposure to chemicals that could lead to intoxication or explosion/fire risk; in particular, this approach will define good laboratory practices and ensure the safety of an operating station. Students will also be trained in the dangers of static electricity, and dust explosions. Finally, students will be introduced to the problem of inerting in chemical reactors and will set up prevention/protection barriers through the use of the What-if method in a process safety approach. The teaching will then be supplemented by the regulatory aspects related to the implementation of REACH, the regulation on explosive atmospheres (ATEX).

***Learning objectives :***
At the end of the course, students must be able to :
- Be able to understand chemical risks (toxicological risks - fire risks) based on physico-chemical properties
- Be able to make exposure scenarios and assess their risks
- Be able to define the inerting processes of chemical reactors
- Perform a workstation analysis

***Prerequisites :***
general chemistry

***Teaching language :*** french
***Documents, website :*** handouts https://coursenligne.chimie-paristech.fr

| 1A<br>S1 | MH11ES.CS | **Solid State Chemistry**<br>*Key words :* ionic model, reticular energy; ionic radius scale, crystal field theory, defects in solids, non stoechiometry |
|---|---|---|

Responsible : Gerard AKA Professeur
gerard.aka@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* written exam integrating a documentary approach |
|---|---|---|---|---|---|
| | 13.50 h | 12 h | 0 h | | |

***Course outline :***
The objective of this teaching is to allow the student to acquire knowledge and skills on the structural description and properties, chemical and physics properties of a crystallized solid. a first part of teaching is devoted to the description of the structural characters of the various ionic solids. The thermodynamics of formation of these solids is then presented. Historical reference marks, relating to the design of the various scales of ionic radius, are mentioned. Models, documents in proof of the variation to the perfect ionic model, are described, followed by the crystal field theory as well as its thermodynamic, structural and magnetic consequences
The model of the perfect crystalline solid is supplemented by the introduction of imperfections or defects existing into all real solids. It is the crystal unit "Perfect + defects" which will form the real solid model. The remarkable properties of the real crystal are presented and discuss in the last part of this teaching.

***Learning objectives :***
At the end of this teaching the student will be able to acquire following knowledge and skills:
1 - To adapt the description of the principal structural types characterizing solids
2 - To know to calculate and interpret the energy of network of a solid
3 - To know how to use the scale of the ionic rays according to Shannon and Prewitt for better understanding the structure of solid
4 - To adapt and analyze the thermodynamic, structural or magnetic consequences related to the existence of crystal field in solids.
5 - To know how to distinguish the various types of intrinsic and extrinsic defects in solids.
6 - To adapt the mechanism of formation of defects in a nonstoechiometric solid and to deduce from them the remarkable. properties (physico chemical) associated with these defects.

***Prerequisites :***
License, Master 1 (L3/M1)

***Teaching language :*** french
***Documents, website :*** Course handout and digital version, visualization software for the structure of crystalline solids, slide show of the course https://coursenligne.chimie-paristech.fr/

| 1A<br>S1 | MH11ES.CDS | **Crystallography**<br>*Key words :* Geometric crystallography, lattices, symmetries, X ray diffraction |
|---|---|---|

Responsible : Gilles Wallez professeur
gilles.wallez@upmc.fr

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* final examination |
|---|---|---|---|---|---|
| | 12 h | 12 h | 0 h | | |

***Course outline :***
Geometric Crystallography describes the crystalline solid through the periodic repetition and the invariance following symmetries of a chemical pattern at lattice points, hence the properties. Beyond, X ray Diffraction is the tool that allows determining the crystal structure at the atomic scale.

***Learning objectives :***
This teaching unit aims at making the student able to apprehend by him/herself the symmetries and the atomic array of a crystal structure. These geometric considerations will be developed in narrow relation with X ray powder diffraction that will allow solving simple crystal structures. In a more general canvas, this unit is linked to teaching in solid state chemistry and is a basis for understanding the properties of materials.

***Prerequisites :***
geometry, trigonometry, scalar and vector products, matrices calculations, complex exponential

***Teaching language :*** french
***Documents, website :*** handouts moodle

| 1A S1 | MH11TC.CE2 | **MANAGEMENT ECONOMIC AND SOCIAL SCIENCES - KNOWLEDGE OF THE COMPANY**<br>*Key words :* engineer, company, management, organization, corporate social responsibility, governance, professional project |
|---|---|---|

Responsible : Philippe Vernazobres et Delphine Bourland Maître de Conférence et enseignante à Chimie ParisTech
philippe.vernazobres@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Summary note on a company + Articulation with the 1A internship where they will be in a participant observation posture |
|---|---|---|---|---|---|
| | 40 h | 0 h | 0 h | | |

***Course outline :***

This UE aims to train and professionalize engineers capable of having a global and transdisciplinary vision of their environment. It is about giving them the tools to enable them to integrate into an organization and to understand the complex challenges of the company.

Course topics - 12h

- The contributions of SHS to the understanding of the company and management (economics, sociology...)
- Engineers and their professions within the organization.
- The major changes in managerial thinking.
- The fundamentals of management: managerial skills and leadership.

Workshop topics - 14h

- Professional project: career path, ambition, French-English CV, cover letters
- Economic approach of the company: definitions, actors, goals, organization, economic, societal and environmental performance
- Governance: awareness of the different modes of governance, identification of stakeholders

Seminar topics - 14h

- Team-building: inclusion-cooperation seminar (7h)
- Corporate Social Responsibility: the responsible engineer, exchanges with professionals (3.5h)
- Round tables: engineering professions, exchanges with professionals (3.5 hours)

***Learning objectives :***

At the end of the modules, the student will be able to:

- Understand basic business vocabulary and concepts
- Understand the reality and complex challenges of the company: economic, social, societal and environmental performance
- Have benchmarks in an organization
- Start getting to know himself, reflect on his career plan, master job search tools

***Prerequisites :***

***Teaching language :*** french

***Documents, website :***

| 1A<br>S1S2 | MH11TC.ANG;<br>MH12TC.ANG; | **GENERAL, SCIENTIFIC AND BUSINESS ENGLISH**<br>*Key words :* English, General, Scientific, Business, Intercultural Skills |
|---|---|---|

Responsible : Daria Moreau Head of Languages and Cultures Department
daria.moreau@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* evaluation reports validation of 5 skills (see CECRL grid) at least at B2 level |
|---|---|---|---|---|---|
| | 0 h | 79.5 h | 0 h | | |

***Course outline :***
These courses are designed to improve English language skills and to teach linguistic autonomy in order to prepare students to work with technical and scientific English in an international or in an intercultural context.
Each student is required to participate in both General and Scientific English classes. The General English courses take place in level groups established at the beginning of the year on the basis of both a placement test and oral evaluations. Students can freely choose the theme-based classes independently on their levels in English. For the most advanced students (bilingual or C2 according to CECRL) it is possible to replace the classroom courses with research work supervised by a teacher from the Department. Low-level students can attend one-to-one tutoring sessions.
The classroom courses are complemented by an adapted and varied "e-learning" (the Yesmag application which aims to facilitate reading texts in their original versions; multiple linguistic activities on Moodle; self-study in the language lab).
General English courses are to master:
- speaking skills: presentations, debates, discussions on cultural topics specific to Anglo-Saxon countries,
- listening and comprehension of TV or radio news,
- synthesis and comparison of authentic documents from the current press,
- CV writing,
- role-playing in professional situations (negotiations, telephone conversations, job interviews),
- analysis of business cases with reference to authentic documents.

Scientific English courses are to:
- work on technical and scientific vocabulary,
- master writing reports, articles, essays,
- practice oral communication on technical, scientific and social subjects,
- discuss scientific articles.

Individual and group project work will also be proposed.

***Learning objectives :***
The student will have a thorough knowledge of grammar and technical/scientific vocabulary to be able to communicate both in written and oral business English in a multicultural company / The student will be prepared to search for an internship or a job in an English-speaking country / The student will write his/her CV in English, taking into account the cultural rules of an English-speaking country / The student will be open to collaborative work / The student will have a strong culture of at least one English-speaking country / The student will learn to master a debate on an everyday life, technical or scientific subject / The student will be able to prepare in advance a clear presentation on a subject with a cultural, civilizational, technical or scientific content / The student will answer factual questions on a given subject / The student will be able to participate in a conversation and express himself/herself on a wide range of topics / The student will synthesize a scientific or general text or an audio, identify relevant information and present it to an audience.

***Prerequisites :*** B1

***Teaching language :*** english
***Documents, website :*** audio and video documents, factual documents https://coursenligne.chimie-paristech.fr/course/view.php?id=76

# SEMESTER 2

| 1A S2 | MH12ES.LC | **Chemical Bonding**<br>*Key words :* chemical bonding |
|---|---|---|

Responsible : Carlo Adamo Professeur
carlo.adamo@chimie-paristech.fr

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Written exam |
|---|---|---|---|---|---|
| | 12 h | 12 h | 0 h | | |

***Course outline :***

This module is an introduction to the main basic concepts encountered in quantum chemistry for the determination of the electronic structure of systems ranging from hydrogen atoms to single multi-electronic molecules.

The main concepts covered are: molecular orbital theory, resolution of the Schrödinger equation, electronic correlation, perturbation or variational approaches, approximate methods for calculating the electronic structure, study of reactivity using boundary orbital theory and characterization of an energy profile.

The training is based on alternating course and TD sessions.

***Learning objectives :***

The student must be able to:

- understand the basic concepts of quantum chemistry
- to be able to describe a multi-electronic atomic or molecular system
- select and use the approximate methods for calculating the electronic structure
- understand the basic concepts of molecular system reactivity

***Prerequisites :***

***Teaching language :*** french

***Documents, website :*** handouts

| 1A<br>S2 | MH12ES.IRM | **Matter-Radiation Interaction**<br>*Key words :* atomic and molecular physics, processes of interaction with radiation |
|---|---|---|

Responsible : Didier Gourier Professeur, Chimie-ParisTech
didier.gourier@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* written examination |
|---|---|---|---|---|---|
| | 15 h | 9 h | 0 h | | |

***Course outline :***
The interaction processes between matter and electromagnetic radiation are the basis of spectroscopic techniques in analytical chemistry as well as major technological applications (imaging techniques, photovoltaics, optoelectronics,...). The objective of the course is to make a general presentation of these processes and to explain the spectroscopic properties in relation to the quantum descriptions of atoms, molecules, and matter in general.

***Learning objectives :***
The student must be able to:
- describe the different ways in which radiation and matter interact,
- describe the different interactions that exist in atoms and molecules,
- to explain the different levels of approximation in the quantum description of atoms and molecules,
- to predict possible transitions in single atoms and molecules and to interpret absorption or emission spectra on this basis.

***Prerequisites :***
Quantum physics, electromagnetism, BSc level

***Teaching language :*** french
***Documents, website :*** https://coursenligne.chimie-paristech.fr

| 1A<br>S2 | MH12FE.IRM | **Practical Work in Spectroscopy: Interaction of Radiation with Matter**<br>*Key words :* quantum mechanics, spectroscopy, signal processing, cristallography, X ray diffraction |
|---|---|---|

Responsible : Loiseau Pascal Maître de Conférences
pascal.loiseau@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* report |
|---|---|---|---|---|---|
| | 0 h | 0 h | 30 h | | |

***Course outline :***
Pratical work about interaction of radiation with matter happens in first year. It focuses on characterization techniques of matter mobilizing knowledge either in crystallography, for the study of any crystallized material, or in spectroscopy based on dipolar electric interactions as well as dipolar magnetic ones, by covering a large range of energy from microwave to visible radiation.
The experimental techniques examined in depth are : X-ray diffraction, electron paramagnetic resonance, Fourier-transform infrared spectroscopy, molecular emission, UV-visible absorption, laser oscillation.

***Learning objectives :***
This practical teaching emphasizes the importance of the operating principles of any experimental techniques on measurement, and applies skills in crystallography-X ray diffraction, interaction of radiation with matter and applied mathematics.
From this practical work, the student will be able to:
- optimize acquisition parameters by considering resolution and signal to noise ratio, in accordance with the signal processing embedded in a measuring equipment
- apply a systematic method of structural analysis, notably by the use of Fullprof software
- identify and classify the nature of electronic transition on a spectrum as a function of energy
- criticize a physical model depending on used hypotheses

***Prerequisites :***
crystallography-X ray diffraction, interaction of radiation with matter, applied mathematics

***Teaching language :*** french
***Documents, website :*** handouts https://coursenligne.chimie-paristech.fr/course/view.php?id=22

| 1A<br>S2 | MH12ES.SR | **Functional groups: synthesis and reactivity**<br>*Key words :* functional group, reactivity, mechanism, multi-step synthesis |
|---|---|---|

Responsible : Pierre HAQUETTE Maître de conférences
pierre.haquette@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Written examination |
|---|---|---|---|---|---|
| | 12 h | 12 h | 0 h | | |

***Course outline :***

The course CMB.SR.1.2 is in continuity with CMB.SR.1.1 and addresses the reactivity of carbonyl functions (aldehydes and ketones) and that of carboxylic acids and their derivatives (additions, oxidation, reduction, enolization, etc.). Particular emphasis is placed on the study of mechanisms by trying to show similarities between seemingly unrelated reactions.

Course program:

1) Organometallic derivatives: preparation, properties
2) Carbonyl derivatives:
   - Nomenclature and physico-chemical properties, preparation
   - Addition reactions (water, alcohols, amines, thiols, etc.)
   - Ylide addition reactions (Wittig, ...)
   - Reduction to alcohol and alkanes
   - Formation and reactivity of enols, enolates, enamines, silylated enol ethers
   - Aldolization, alkylation, halogenation
   - Michael's Additions, Robinson's Annellation
   - Oxidation and reduction reactions
3) Carboxylic acids and derivatives:
   - Nomenclature and physico-chemical properties, preparation of acids and derivatives
   - Curtius, Arndt Eistert, Knoevenagel, Darzens reactions
   - Wolff's rearrangement,
   - Claisen and Dieckman condensation
   - Reduction reactions

***Learning objectives :***

By the end of the EU CMB.SR.1.2, students will have acquired the basics of organic chemistry as a tool for the development of synthesis processes. They will be in possession of the knowledge necessary to understand and analyze the mechanisms of the main reactions that lead to organic compounds. They will be able to apply these concepts to the resolution of simple synthesis and retrosynthesis problems.

***Prerequisites :***

Basic course in organic chemistry (preparatory class, L2)

***Teaching language :*** french
***Documents, website :*** handouts

| 1A<br>S2 | MH12FE.CMB | **Experimental training in molecular chemistry**<br>*Key words :* |
|---|---|---|

Responsible : Sylvain Darses
sylvain.darses@chimie-paristech.fr

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* report and laboratory behavior |
|---|---|---|---|---|---|
| | 0 h | 0 h | 60 h | | |

***Course outline :***
In this laboratory experimental work module, through multi-step syntheses in relation with the course and the tutorials, the students approach the classic techniques of synthesis and purification and put into practice the knowledge acquired in the spectroscopy module (IR , NMR, ...) to analyze the synthesized compounds. Students are gradually brought to work autonomously, to determine themselves, by means of a bibliographical research, the most suitable synthesis routes and to implement them. This work is the subject of a professional situation (compliance with the rules of hygiene and safety and implementation of special measures, keeping a laboratory notebook, writing reports).

***Learning objectives :***
The objective of this practical work is to train engineering students in the basic techniques of organic synthesis (conventional assemblies, low-temperature reactions, reactions under inert atmosphere, distillation, recrystallization, column chromatography, etc.). analysis (GC, FT-IR, NMR, ...) and raise awareness of health and safety issues.

***Prerequisites :***
none

***Teaching language :*** french
***Documents, website :*** handouts

| 1A S2 | MH12ES.GC | **Chemical Engineering**<br>*Key words :* fluid mechanics , mass and heat transfer, unit operations of fluid mixtures |
|---|---|---|

Responsible : Frédéric ROUSSEAU Enseignant-Chercheur
frederic.rousseau@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* written exam with documents and calculators |
|---|---|---|---|---|---|
| | 19.5 h | 4.5 h | 30 h | | |

***Course outline :***

This training aims to present the steps to follow to control the operation of a process of transformation of the material with or without chemical reactions.

A chemical process consists of a reactor in which the chemical reactions take place, and downstream of the devices (distillation, extraction, etc.) intended to separate and / or purify the products obtained. Depending on the application sought, we operate with a continuous or discontinuous process .

In the face of this complexity, the first step is to understand the transfer processes at the local scale: the mechanics of moving fluids, the energy transfer and in particular the heat transfer (conduction, convection and radiation) and finally the transfer of matter in mono-phasic and bi-phasic media.

To optimize these transfer processes, very often coupled, steady state or transient software are made available to students in TP. To simulate the operation of the process, the equation of processes is necessary and the resolution of the equation system is possible thanks to the computer. Thus, if the use of mathematics is a means and not an end, the mathematical tool is unavoidable. It must be understood and mastered so that these programs are not black boxes. The course and TD sessions are devoted to understanding the concepts involved. This approach is complemented by experimental teaching in the laboratory on pilots which allows to compare theory and practice.

All this information is recorded in 2 books recently published by the teachers and made available to each student. This knowledge and know-how is very useful and essential to understand the operation of a process in research, development or production in an academic or industrial environment.

***Learning objectives :***

At the end of this training the student understands that the access to the economic balance of a process or to the optimization of a manufacturing unit it is necessary to know the balance material and energy. The student then has the skills to adapt to economic constraints (produce added value, respect the environment, seek energy efficiency ...)

The adjustment of the parameters of a process, often dependent, is not empirical but the result of a rigorous scientific analysis. Under these conditions the process is adaptable to economic constraints.

Thus the thermodynamic analysis of transfers and phase equilibria informs about what is possible. Kinetic analysis and balance sheets make it possible to check if the choice is reasonable. This gives access to the cost of operation Finally, the data obtained make it possible to calculate the sizing of the units (reactors, distillation, L-L extraction, absorption, etc.) to quantify the investment.

***Prerequisites :***

thermodynamic solutions / partial derivatives

***Teaching language :*** french

***Documents, website :*** books, Power Points www.editions-ellipses.fr

| 1A<br>S2 | MH12FE.GC | **EXPERIMENTAL TRAINING IN CHEMICAL ENGINEERING**<br>*Key words :* heat and mass transfer, unit operation, simulation |
|---|---|---|

Responsible : Mengxue Zhang
mengxue.zhang@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Continuous monitoring :written reports and oral presentation |
|---|---|---|---|---|---|
| | 0 h | 0 h | 30 h | | |

***Course outline :***
The practical work followed by each engineering student must help to apply the concepts developed in class and in tutorials (unit operations and heat transfers) and to complete their experimental training in fluid mechanics. The work is carried out in pairs and must be reported both in written or oral forms.

***Learning objectives :***
To give the future engineer a knowledge base, complementary to his training in fluid mechanics and heat transfer (Fourier's law). For the future engineer, this will be:
- To be able to describe and estimate pressure drops in a network where a fluid flows.
- Define, explain and determine the different types of heat transfer
- Be able to describe the phenomena involved in unit operations and to dimension such a system.
- Acquire notions of simulation on Chemical Engineering software

***Prerequisites :***

***Teaching language :*** french
***Documents, website :*** handouts https://coursenligne.chimie-paristech.fr/enrol/index.php?id=21

| 1A<br>S2 | MH12ES.MN | **Numerical methods**<br>*Key words :* Algorithmics, programming, C |
|---|---|---|

Responsible : Frédéric Labat Maître de Conférences
frederic.labat@chimie-paristech.fr

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Written report |
|---|---|---|---|---|---|
| | 0 h | 26 h | 0 h | | |

***Course outline :***
This module aims to train the engineering student in the classical techniques of numerical methods commonly encountered in various scientific fields, in order to enable him/her to choose an algorithm adapted to a given problem and to implement it by making an application in C language.
The algorithms introduced cover problems regularly encountered in various scientific fields, such as the solution of linear and non-linear equations, derivation and numerical integration, the calculation of eigenvalues and vectors, the minimization of functions, the solution of differential equations or partial differential equations.
Particular attention is paid to the efficiency, quality and limitations of the IT solutions that can be used.
The training is based on course/TD sessions, based on examples mainly taken from the field of chemistry, using the free software Code::Blocks, easily installed on any personal computer.

***Learning objectives :***
The student must be able to:
- analyze a scientific problem and determine the appropriate numerical methods for its resolution
- implement the main resolution algorithms
- analyze with a critical mind the results obtained, aware of the limits of the methods used

***Prerequisites :***
C programming : basics

***Teaching language :*** french
***Documents, website :*** handouts

| 1A<br>S2 | MH12ES.CS | **Solution chemistry**<br>*Key words :* Chemistry of aqueous and non-aqueous solutions, chemical separations, complexation, solubilization, precipitation, extraction |
|---|---|---|

Responsible : Varenne Anne Professeur
anne.varenne@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Article study, multiple choice questions, and terminal exam |
|---|---|---|---|---|---|
| | 7.5 h | 4.5 h | 0 h | | |

***Course outline :***
Aqueous solutions :
- Diluted, concentrated, complex solutions
- Activity, activity coefficient (Debye and Hückel models, Davies, Theory of specific interactions, Pitzer model).
- Complexing: successive or global formation constants, complexing coefficient, distribution diagram, action of acidity on the complexing coefficients.
- Types of ligand (H, OH, L), multi-ligand complexation,.....

Chemical separations :
- Solubilization / precipitation
- Liquid/liquid extraction: principle, simple or complex equilibria
- Extraction phenomenon: co-extraction / ion exchange
- Synergism, release
- Liquid/solid extraction: ion exchange resins, distribution equilibria, complexing effect

Non-aqueous reaction media:
- Micellar media (presentation, micelles for separations, three-phase system, cloud point, liposomes, microemulsions for extraction)
- Molecular solvents (solvation, acid-base properties, ion pairs...)
- Molten salt media: molten salts at high temperature (presentation, oxoacidity, extraction applications) and ionic liquids (presentation, some properties, extraction applications)
- Supercritical fluids (presentation, some properties, extraction applications)

Articles are studied and criticized.

***Learning objectives :***
Understanding and control of solution interactions for the purpose of separating and samples treatment in complex matrices.
The applications presented are varied with an emphasis on nuclear and environmental issues.

***Prerequisites :***
Solvents, acidity in aqueous medium, properties of ions, simple complexation, basic notions of electrochemistry

***Teaching language :*** french
***Documents, website :*** handouts in french, articles in english

| 1A<br>S2 | MH12ES.MS | **Separation Sciences**<br>*Key words :* chromatography, capillary electrophoresis, solid phase extraction, sample preparation, analytical separation |
|---|---|---|

Responsible : d'Orlyé Maître de conférences
fanny.dorlye@chimieparistech.psl.eu

| *ECTS :* | *Course*<br>6 h | *Tutorials*<br>6 h | *Practical work* | *Mentoring* | *Evaluation method :* continuous control (MCQs and participation) and a final written exam with documents |
|---|---|---|---|---|---|

***Course outline :***
Generalities on chromatographic separation methods: principles (interactions and separations), purposes, classification of methods, thin layer and column implementation, instrumental aspects, fields of application Chromatographic interactions and physico-chemical mechanisms controlling separations: volatility, differential interactions, choice of stationary and mobile phases Fundamental quantities and optimization parameters : Retention magnitudes, selectivity, dispersion, resolution On-line and coupled detections to chromatographs: characteristics of detectors, main detection modes, application to qualitative and quantitative analysis (calibration methods) Comparison of liquid and gas chromatography and positioning of chromatographic methods in relation to other separative methods. Introduction to capillary electrophoresis.

***Learning objectives :***
The aim of this course is to introduce 1st year students to analytical chromatographic methods before they start practicing in laboratory classes or internships. At the end of this course the students should have a good overview of the different chromatographic approaches and their fields of application. They should have enough knowledge on technological and methodological elements to implement all types of chromatography and optimize separation performances from an analytical point of view.

***Prerequisites :***
Basics of thermodynamics, solution chemistry, spectroscopy, analytical chemistry, organic chemistry, hydrodynamics, mathematical

***Teaching language :*** french
***Documents, website :*** handouts, self evaluation quiz, simulation software

| 1A<br>S2 | MH12ES.EC | **Analytical electrochemistry, from mechanisms to applications**<br>*Key words :* Electrochemistry, microelectrolysis, voltammetry, analysis, effect of the chemical medium, electrochemical kinetics, generators |
|---|---|---|

Responsible : Michel Cassir Professeur
michel.cassir@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* A final exam (80%) + a project (20%) |
|---|---|---|---|---|---|
| | 15 h | 9 h | 0 h | | |

***Course outline :***

This course is addressed to engineer students that already have some notions on electrochemical potentials. As a first step, we will describe the fundamental principles of electrochemistry at equilibrium, in particular microelectrolysis and the current-potential characteristics I=f(E), that constitute a basis for the approach in analysis and the comprehension of mass and charge transfer at the electrodes. We will largely introduce the effect of the chemical medium on I=f(E) curves. Afterwards, we will develop the notions of electrochemical kinetics and coupled reaction to charge transfer, through cyclic voltammetry that enables to analyse electrochemical processes with short lifetime. We will finally give a panorama of the applications of electrochemistry to electrolysis and electrochemical generators, such as fuel cells and batteries.

***Learning objectives :***

- The student will be able to understand the fundamental aspects of electrochemistry;
- He will understand the interest and implementation of microelectrolysis;
- He will know how to establish equations of current-potential characteristics under equilibrium conditions;
- He will integrate the effect of the chemical medium (acidity, complexation, precipitation) in the establishment and plot of I = f (E) curves;
- He will assimilate the basic equations of electrochemical kinetics;
- He will be able to interpret the reactions coupled to charge transfer through cyclic voltammetry.
- He will have basic knowledge and good vision of the applications of electrochemistry to electrolysis and electrochemical generators.

***Prerequisites :***

Notions on electrochemical potentials end equilibria, basis in thermodynamics and solution chemistry

***Teaching language :*** french
***Documents, website :*** pdf documents, handouts

| 1A<br>S2 | MH12TC.CE | **MANAGEMENT ECONOMIC AND SOCIAL SCIENCES - KNOWLEDGE OF THE COMPANY - Intro. to economics and innovation management**<br>*Key words :* innovation, design thinking, entrepreneurship, intellectual property, sustainable dvp, market, circuit, return on investment |
|---|---|---|

Responsible : Philippe Vernazobres Maître de Conférences Chimie ParisTech
philippe.vernazobres@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Final written evaluation for economics and conferences + Industrial jury for innovation week |
|---|---|---|---|---|---|
| | 42 h | 0 h | 0 h | | |

***Course outline :***

This EU aims to train engineers capable of innovating and understanding the economic environment and the challenges facing the company.

Economics course topics - 7.5 hours
- Purpose of the economic analysis and basic concepts : markets, prices
- Introduction to macroeconomic analysis: circuits, basic concepts
- Introduction to the economic analysis of money
- Introduction to the logic of calculating investment profitability

Topics of managerial conferences (examples) + preparation for the internship - 10.5 hours
- Sustainable development economics, energy transition and CSR
- Business intelligence, crisis communication
- Entrepreneurship
- Patents and intellectual property protection

Innovation Week - 24.5h
- Creativity and innovation seminar with design thinking (2 days)
- Visit of the Chimie ParisTech research laboratories (1 day)
- Conferences (1/2 day)

***Learning objectives :***

At the end of the modules, the student will be able to:
- Understand the basic mechanisms of economics
- Understand the managerial subjects essential to the engineer
- To be involved in an innovation process, the core business of engineers, modules extended in the 2nd and 3rd year
- Experiment and understand a design thinking approach, cooperate in a team
- Defend an innovative project in competition before an industrial jury

***Prerequisites :***

***Teaching language :*** french
***Documents, website :*** handouts

| 1A<br>S2 | MH12TC.PTD | **Transdisciplinary project**<br>*Key words : Team, project management, project manager, planning, deadlines, specifications, deliverable, customer relationship.* |
|---|---|---|

Responsible : Philippe Vernazobres
philippe.vernazobres@chimieparistech.psl.eu

| *ECTS :* | *Course*<br>h | *Tutorials*<br>h | *Practical work*<br>h | *Mentoring* | *Evaluation method :* Writing a project report and oral defense |
|---|---|---|---|---|---|

***Course outline :***

This module consists in putting students in a teamwork condition in project mode to enable them to acquire the methods and postures of project management.

The work is organized in groups of seven for one semester (January-June), half a day a week. It deals with real subjects proposed by industrial and institutional clients. These subjects focus on transversal themes: technological and/or social, societal and environmental dimensions. The groups are tutored by teacher-researchers from the school, and the students experiment in a rotating way with the posture of project leader. Conferences provide project management tools and processes.

***Learning objectives :***

At the end of the module, the student will be able to:

- Work in a team and open up to the practice of collaborative work.
- Manage the relationship with a client, from demand analysis to project delivery.
- Organize, plan a project, respect deadlines and develop specifications.
- Assume the role of project manager.
- Identify, model and solve unusual and incompletely defined problems.
- Take into account the transversal challenges of companies and society (economic, social, ethical, environmental...) and develop a critical spirit and approach to these challenges.
- Take into account the issues of labour relations, ethics and social responsibility at work.
- Find relevant information to respond to the customer's request, evaluate and implement it.
- Report on this experience and produce a deliverable, both written (report) and oral (presentation to clients).)

***Prerequisites :***

***Teaching language :*** french

***Documents, website :***

| 1A<br>S2 | MH12ST.SDE | **INTERNSHIP TO DISCOVER THE COMPANY**<br>*Key words :* company, work organization, organization chart, labour relations, corporate social responsibility, safety |
|---|---|---|

Responsible : Philippe Vernazobres Maître de Conférence à Chimie ParisTech
philippe.vernazobres@chimieparistech.psl.eu

| *ECTS :* | *Course* | *Tutorials* | *Practical work* | *Mentoring* | *Evaluation method :* Internship report |
|---|---|---|---|---|---|
| | 0 h | 150 h | 0 h | | |

***Course outline :***
Internship of one to two months, of first discovery of the company as a worker or technician.
It is a question of being part of a participatory observation logic in order to, on the one hand, carry out field work and, on the other hand, communicate in writing to report on this experience in a professional way.
The internship report:
- mobilizes first year management courses to situate themselves in the company and understand its challenges.
- Invites to observe the organization of human resources, which will be the subject of management courses in the second year.

***Learning objectives :***
At the end of the internship, the student will be able to:
- Integrate and position him/herself in an organization
- Be an actor and responsible for the tasks entrusted to him/her
- Observe and take a step back on the organization, labour relations, productivity, quality, safety, sustainable development, the environment...
- Report this experience regarding to :
o the company's challenges
o the tasks performed
o the construction of the professional project : knowing yourself, making choices

***Prerequisites :***
Management modules for the 1st and 2nd semester

***Teaching language :*** french
***Documents, website :*** grid for writing the internship report