

**PEOPLE'S DEMOCRATIC REPUBLIC OF ALGERIA**

**MINISTRY OF HIGHER EDUCATION AND SCIENTIFIC RESEARCH**

# **The Chemistry Bachelor's programme**

<b>Establishment</b>	<b>Faculty / Institute</b>	<b>Department</b>
<b>University of Djilali Bounaama de Khemis Miliana</b>	<b>Faculty of Science</b>	<b>Science of matter</b>

<b>Field</b>	<b>Branch</b>	<b>Speciality</b>
<b>SCIENCE OF THE MATER</b>	<b>Chemistry</b>	<b>Fundamental Chemistry</b>

**Bachelor in Branch: Chemistry**  
**Speciality: Fundamental Chemistry**

***Summary of objectives and training pathways in a paragraph not exceeding 5 lines (in English)***  
***(In English)***

The license in fundamental chemistry is academic type training. This license is designed as a set of educational units whose purpose is to give the students concerned a solid training in organic chemistry, analytical chemistry, quantum chemistry, as well as physical chemistry (thermodynamics of solutions, surface chemistry and catalysis and electrochemistry) and crystallography.

# **I – Half-yearly lesson organization sheet**

## 1-Semester 3

Teaching unit	WHV	H.V weekly			Others * (14-16 sem)	Coeff	Credits	Assessment method	
	14-16 week	C	tutorials	PW				CM	Exam
<b>TE fundamental</b>									
<b>TUF3</b>	<b>225h00</b>	<b>9h00</b>	<b>6h00</b>		<b>275h00</b>	<b>10</b>	<b>20</b>	<b>33%</b>	<b>67%</b>
Mineral Chemistry	67h30	3h00	1h30	-	82h30	3	6	33%	67%
Organic Chemistry 1	67h30	3h00	1h30	-	82h30	3	6	33%	67%
Applied mathematics	45h00	1h30	1h30	-	55h00	2	4	33%	67%
Vibrations, Waves and Optics	45h00	1h30	1h30	-	55h00	2	4	33%	67%
<b>TU methodology</b>									
<b>TUM3</b>	<b>90h00</b>	<b>1h30</b>		<b>4h30</b>	<b>85h00</b>	<b>4</b>	<b>7</b>	<b>50%</b>	<b>50%</b>
Inorganic Chemistry Practical Work	22h30	-	-	1h30	27h30	1	2	50%	50%
Organic Chemistry Practical Work	22h30	-	-	1h30	27h30	1	2	50%	50%
Numerical Methods and Programming	45h00	1h30	-	1h30	30h00	2	3	50%	50%
<b>TU discovery</b>									
<b>TUD3</b>	<b>45h00</b>	<b>1h30</b>	<b>1h30</b>		<b>5h00</b>	<b>2</b>	<b>2</b>		<b>100%</b>
Physico-Chemical Analysis Techniques I	45h00	1h30	1h30	-	5h00	2	2	-	100%
<b>UE transversal</b>									
<b>TUT3</b>	<b>15h00</b>	<b>1h00</b>			<b>10h00</b>	<b>1</b>	<b>1</b>		<b>100%</b>
Foreign languages 3	15h00	1h00	-	-	10h00	1	1	-	100%
<b>Total Semester 3</b>	<b>375h00</b>	<b>13h00</b>	<b>7h30</b>	<b>4h30</b>	<b>375h00</b>	<b>17</b>	<b>30</b>		

\* Other = Additional work in semester consultation (personal work of the student)

## 2-Semester 4

Teaching unit	WHV	H .V weekly			Others * (14-16 sem)	Coeff	Credits	Assessment method	
	14-16 week	C	tutori als	PW				CM	Exam
<b>TU fundamental</b>									
<b>TUF4</b>	<b>202h30</b>	<b>7h30</b>	<b>6h00</b>		<b>247.30</b>	<b>10</b>	<b>20</b>	<b>33%</b>	<b>67%</b>
<b>Organic Chemistry 2</b>	67h30	3h00	1h30	-	82h30	3	6	33%	67%
<b>Thermodynamics and Chemical Kinetics</b>	67h30	3h00	1h30	-	55h00	3	6	33%	67%
<b>Analytical Chemistry</b>	45h00	1h30	1h30	-	55h00	2	4	33%	67%
<b>Quantum Chemistry</b>	45h00	1h30	1h30	-	55h00	2	4	33%	67%
<b>TU methodology</b>									
<b>TUM 4</b>	<b>112h30</b>	<b>3h00</b>		<b>4h30</b>	<b>87h30</b>	<b>5</b>	<b>8</b>	<b>50%</b>	<b>50%</b>
<b>Analytical Chemistry Practical Work</b>	22h30	-		1h30	27h30	1	2	50%	50%
<b>Practical work in thermodynamics and Chemical Kinetics</b>	45h00	1h30		1h30	30h00	2	3	50%	50%
<b>Inorganic Chemistry</b>	45h00	1h30		1h30	30h00	2	3	50%	50%
<b>TU discovery</b>									
<b>TUD4</b>	<b>45h00</b>	<b>1h30</b>	<b>1h30</b>		<b>05h00</b>	<b>2</b>	<b>2</b>		<b>100%</b>
<b>Techniques of Physico-chemical Analysis II</b>	45h00	1h30	1h30	-	05h00	2	2		100%
<b>TU transversal</b>									
<b>TUT4</b>	<b>15h00</b>	<b>1h00</b>			<b>10h00</b>	<b>1</b>	<b>1</b>		<b>100%</b>
<b>Foreign languages 4</b>	15h00	1h00	-	-	10h00	1	1		100%
<b>Total Semester 4</b>	<b>375h00</b>	<b>13h00</b>	<b>7h30</b>	<b>4h30</b>	<b>375h00</b>	<b>17</b>	<b>30</b>		

\* Other = Additional work in semester consultation (personal work of the student)

### 3-Semester 5 :

Teaching unit	WHV	H .V weekly				Coeff	Credits	Assessment method	
	14-16 week	C	tutorials	P W	Others * (14-16 sem)			CM	Exam
<b>TU fundamental</b>									
<b>TUF5.1</b>	<b>135h00</b>	<b>9h00</b>	<b>3h00</b>		<b>105h00</b>	<b>6</b>	<b>10</b>	<b>33%</b>	<b>67%</b>
Organic Chemistry III	67 h30	3h00	1h30		52 h30	3	5	33 %	67 %
Analytical Chemistry II	67 h30	3h00	1h30		52 h30	3	5	33 %	67 %
<b>TUF5.2</b>	<b>135h00</b>	<b>9h00</b>	<b>3h00</b>		<b>105h00</b>	<b>6</b>	<b>10</b>	<b>33%</b>	<b>67%</b>
Crystallography	67h30	3h00	1h30		52h30	3	5	33 %	67 %
Quantum Chemistry II	67h30	3h00	1h30		52h30	3	5	33 %	67 %
<b>TU methodology</b>									
<b>TUM5</b>	<b>25h00</b>			<b>3h00</b>	<b>105h00</b>	<b>4</b>	<b>6</b>	<b>50 %</b>	<b>50 %</b>
PW Analytical chemistry	22h30			1h30	52h30	2	3	50 %	50 %
PW Molecular modeling	22h30			1h30	52h30	2	3	50 %	50 %
<b>TU discovery</b>									
<b>TUD5</b>	<b>22h30</b>	<b>1h30</b>			<b>27h30</b>	<b>1</b>	<b>2</b>		<b>100 %</b>
Environmental Chemistry	22h30	1h30			27h30	1	2		100 %
<b>TU transversal</b>									
<b>TUT5</b>	<b>22h30</b>	<b>1h30</b>			<b>27h30</b>	<b>1</b>	<b>2</b>		<b>100 %</b>
Scientific English I	22h30	1h30			27h30	1	2		100 %
<b>Total Semestre 5</b>	<b>360 h</b>	<b>15 h</b>	<b>6 h</b>	<b>3h00</b>	<b>360 h</b>	<b>18</b>	<b>30</b>		

*\* Other = Additional work in semester consultation (personal work of the student)*

## 4- Semester 6:

Teaching unit	WHV	H . V weekly				Coeff	Credits	Assessment method	
	14-16 week	C	tutorials	PW	CM*			CM	Exam
<b>TU fundamental</b>									
<b>TUF6.1</b>	<b>135h00</b>	<b>9h00</b>	<b>3h00</b>		<b>105h00</b>	<b>6</b>	<b>10</b>	<b>33%</b>	<b>67%</b>
Thermodynamics of solutions	67h30	3h00	1h30		52h30	3	5	33 %	67 %
Electrochemistry	67h30	3h00	1h30		52h30	3	5	33 %	67 %
<b>TUF6.2</b>	<b>135h00</b>	<b>9h00</b>	<b>3h00</b>		<b>105h00</b>	<b>6</b>	<b>10</b>	<b>33%</b>	<b>67%</b>
Molecular spectroscopy	67h30	3h00	1h30		52h30	3	5	33 %	67 %
Surface chemistry and catalysis	67h30	3h00	1h30		52h30	3	5	33 %	67 %
<b>TU methodology</b>									
<b>TUM6</b>	<b>25h00</b>			<b>3h00</b>	<b>105h00</b>	<b>4</b>	<b>6</b>	<b>50 %</b>	<b>50 %</b>
Practical work in Electrochemistry	22h30			1h30	52h30	2	3	50 %	50 %
Practical work Physico-chemical methods	22h30			1h30	52h30	2	3	50 %	50 %
<b>TU discovery</b>									
<b>TUD6</b>	<b>22h30</b>	<b>1h30</b>			<b>27h30</b>	<b>1</b>	<b>2</b>		<b>100 %</b>
Ethics and deontology	22h30	1h30			27h30	1	2		100 %
<b>TU transversal</b>									
<b>TUT6</b>	<b>22h30</b>	<b>1h30</b>			<b>27h30</b>	<b>1</b>	<b>2</b>		<b>100 %</b>
Scientific English II	22h30	1h30			27h30	1	2		100 %
<b>Total Semester 6</b>	<b>360 h</b>	<b>15 h</b>	<b>6 h</b>	<b>3 h</b>	<b>370 h</b>	<b>18</b>	<b>30</b>		

*\* Other = Additional work in semester consultation (personal work of the student)*

## **II –Detailed program by subject of semesters**



**Semester: 3**

**TU fundamental**

**Course: Inorganic Chemistry**

**Course content:**

**Chapter 1: Periodic Table**

1. Elements in the periodic table (groups, periods, periodicity of properties)
2. Families of elements (alkali metals, alkaline earth metals, transition metals, halogens, carbon and group IVA elements, nitrogen and group VA elements, oxygen and group VIA elements)
3. Chemical bonding:
  - Covalent bonding
  - Ionic bonding
  - Metallic bonding
  - Van der Waals and hydrogen bonding
4. Molecular orbital energy diagram
5. Hybridization
6. Polarization of a bond

**Chapter 2: Complexes**

1. Concepts of complex (ligands, complexing agents)
2. Study of chemical bonding in complexes, hybridizations in complexes
3. Structures of coordination complexes
4. Properties of complexes
5. Crystal field theory
6. Reactivity of complexes, applications
7. Nomenclature

**Chapter 3:** Hydrogen Natural state, physicochemical properties, preparation of hydrogen, hydrogen compounds (hydrides, hydrogen halides)

**Chapter 4:** Oxygen Natural state, physicochemical properties, preparation, use, oxygen-based compounds, reactivity of oxygen

**Chapter 5:** Halogens (F, Cl, Br, I) In all cases, we will study the natural state, physicochemical properties, preparation, and use.

**Chapter 6:** Sulfur Natural state, properties, preparation, sulfur compounds, hydrogen sulfide, production of sulfuric acid and its use.

**Chapter 7:** Nitrogen Natural state, physicochemical properties, preparation, ammonia and its properties, nitrogen oxides and oxacids. Preparation of nitric acid and its use.

**Chapter 8:** Phosphorus, arsenic, and antimony Natural states of these elements, their preparation, and use

**Chapter 9:** Silicon Physicochemical properties, preparation, silicon oxides and oxacids, silicates, silica gel, silicones.

## Chapter 10: Metals

- Alkali metals: group I of the periodic table: generalities, properties. Sodium: manufacturing, sodium derivatives.
- Aluminum: properties, natural state, preparation, use.
- Iron: natural state, properties, preparation, and use.

### Bibliographic references

- P. W. ATKINS, D.F. SHRIVER, *Chimie inorganique*, Ed. De Boek, (2001)
- C. E. HOUSECROFT, A. G. SHARPE, *Chimie inorganique*, Tr. A. Pousse, Ed. De Boek, (2010)
- R. DIDIER, P. GRECIAS, *Chimie Générale, cours et exercices résolus*, Tec & Doc,(2004).
- S. S. ZUMDAHL, *Chimie générale*, De Boeck, (1999)
- C. E. HOUSECROFT, A. G. SHARPE, *Inorganic chemistry*, 2<sup>nd</sup> Ed. De Boek, (2005)

**Semester: 3**

**TE fundamental**

**Course: Organic Chemistry 1**

**Course Content:**

**Chapter 1: Chemical Bonding**

Recalls on atomic orbitals, Intramolecular bonds, Covalent bond, Carbon hybridization ( $sp^3$ ,  $sp^2$ ,  $sp$ ), VSEPR method, Ionic bond. Intermolecular bonds (hydrogen bonding)

**Chapter 2: Organic Compounds**

Classification of main chemical functions. Nomenclature. Introduction to "ChemDraw" software.

**Chapter 3: Structural Effects**

Electronic effects, Sigma bond polarization, Inductive effect, Electron delocalization in pi bonds (study of 1,3-butadiene and benzene molecules), Consequence of pi bond electron delocalization, Mesomerism and resonance. Steric effects. Consequence of structural effects on the acidity and basicity of an organic compound.

**Chapter 4: Isomerism**

Plane isomerism (or constitutional isomerism), Functional isomerism, Position isomerism, Chain isomerism, Tautomerism. Stereochemistry, Perspective or cavalier representation, Projective representation (Cram's convention), Fischer projection, Newman projection. Stereoisomerism, Conformational isomers (or conformers), ethane, cyclohexane, Configurational isomers (Chirality concept, Optical activity, R,S nomenclature, CIP sequence rules (Cahn, Ingold, and Prelog), Fischer D,L nomenclature, Erythro-threo nomenclature).

**Chapter 5: Diastereoisomerism**

Sigma diastereoisomers due to asymmetric carbons, Pi diastereoisomers (geometric isomerism, Z/E, Cis/trans)

**Chapter 6: Study of Reaction Mechanisms**

Reaction intermediates, Role of solvent (polar, nonpolar), Bond breaking (formation of radicals, carbocations, carbanions), Electrophilic and nucleophilic reagents. Kinetic and energetic aspects of reactions. Study of main reaction mechanisms, Addition reactions: Electrophilic addition, Radical addition, Nucleophilic addition, Substitution reactions: Nucleophilic substitution  $SN_1$  and  $SN_2$ ; Radical substitution; Electrophilic substitution, Elimination reaction  $E_1$ ,  $E_2$ .

**Bibliographic references**

- P. ARNAUD. *Cours : Chimie organique*, 18<sup>ème</sup> éd. Dunod, (2009).
- P. ARNAUD. *Exercices de chimie organique*, 4<sup>ème</sup> éd. Dunod, (2010).
- K.P.C. VOLLHARDT, N. E. SCHORE, C. ESKENAZI. *Traité de chimie organique*, 5<sup>ème</sup> éd. DeBoeck Université, (2009).
- J. McMURRY, E. SIMANEK. *Chimie organique Les grands principes -Cours et exercices corrigés*. 2<sup>ème</sup> éd., DUNOD, (2007).

**Semester: 3**

**TE fundamental**

**Course: Applied Mathematics**

**Course Content:**

**Chapter 1:** Single and Multiple Integrals (2 weeks)

Review of Riemann integral and calculation of primitives. Double and triple integrals. Applications to the calculation of areas, volumes, etc.

**Chapter 2:** Improper Integrals (2 weeks)

Integrals of functions defined on an unbounded interval. Integrals of functions defined on a bounded interval, infinite at one end.

**Chapter 3:** Differential Equations (2 weeks)

Ordinary differential equations of the 1st and 2nd order. Elements of partial differential equations.

**Chapter 4:** Series (3 weeks)

Numerical series. Sequences and series of functions. Power series, Fourier series.

**Chapter 5:** Laplace Transform (3 weeks)

Definition and properties. Application to the resolution of differential equations.

**Chapter 6:** Fourier Transform (3 weeks)

Definition and properties. Application to the resolution of differential equations.

**Bibliographic references**

- J. M. RAKOSOTON, J. E. RAKOSOTON, *Analyse fonctionnelle appliquée aux équations aux dérivées partielles*, Ed. PUF, (1999).
- S. NICAISE, *Analyse numérique et équations aux dérivées partielles : cours et problèmes résolus*, Ed. Dunod, Paris, (2000).
- Elie BELORIZKY, *Outils mathématiques à l'usage des scientifiques et des ingénieurs*, EDP Sciences, Paris, (2007).
- C. ASLANGUL, *Des mathématiques pour les sciences, Concepts, méthodes et techniques pour la modélisation*, De Boeck, Bruxelles (2011).
- C. ASLANGUL, *Des mathématiques pour les sciences2*, Corrigés détaillés et commentés de exercices et problèmes, De Boeck, Bruxelles (2013).

**Semester : 3**

**TE fundamental**

**Course: Vibrations, Waves & Optics**

**Course Content:**

## **PART I: VIBRATIONS**

### **Chapter 1: Free Oscillator.**

Definition of vibrational motion, condition for oscillations, examples of oscillating systems. Definition of a free oscillator, establishment of the equation of motion (Newton's Second Law), harmonic motion equation, energy analysis.

### **Chapter 2: Damped Oscillator.**

Types of friction, definition of a damped oscillator, establishment of the equation of motion (Newton's Second Law), harmonic motion equation, energy analysis.

### **Chapter 3: Forced Oscillator.**

Definition of a forced oscillator, establishment of the equation of motion, harmonic motion equation (Newton's Second Law), resonance. Mechanical/electrical oscillator analogy.

### **Chapter 4: Lagrange method and systems with 2 degrees of freedom.**

Definition of the Lagrangian of a system. Presentation of Lagrange's equations. Definition of the number of degrees of freedom. Application to a system with one degree of freedom. Application to a system with two degrees of freedom.

## **PART II: WAVES**

### **Chapter 5: Progressive Waves.**

Definition of a progressive wave. Conditions for the existence of a wave. Characteristics of a wave. Establishment of the wave propagation equation (vibrating string). Energy carried by a progressive wave.

### **Chapter 6: Standing Waves.**

Definition of a standing wave and fixed boundary conditions. Energy contained in a standing wave.

## **PART III: OPTICS**

### **Chapter 7: Reflection and Refraction of Light.**

Approximation of the light ray. Law of reflection (Snell-Descartes). Law of refraction. The prism.

### **Chapter 8: Formation of Images.**

Stigmatism. Gauss's approximation. Plane and spherical surfaces. Plane and spherical mirrors. Thin lenses.

### **Bibliographic references**

- T. BECHERRAWY, *Vibrations et Ondes*, Tomes 1-4, (Ed. Hermes-Lavoisier - 2010).
- H. DJELOUAH, *Vibrations et Ondes Mécaniques*, OPU, (2011).
- J. BRUNEAUX, *Vibrations et Ondes*, (Ed. Marketing- 2010).

**Semester: 3**

**UE: Methodology**

**Course: Practical Work in Inorganic Chemistry**

### **Course Content:**

**Carry out 5 experiments of your choice.**

1. Concepts of salts in solution
2. Solubility-complex
3. Redox reactions
4. Formation of complexes
5. Solubility product of lead chloride
6. Selective precipitation of barium sulfate and calcium sulfate.

### **Bibliographic references**

- T. BARILERO, A. DELEUZE, M. EMOND, H. MONIN-SOYER, *Travaux pratiques de chimie, de l'expérience à l'interprétation*, Ed. Rue d'ULM, (2013)

**Semester: 3**

**UE: Methodology**

**Course: Organic Chemistry Laboratory Work**

**Course Content:**

Perform 5 or 6 experiments, depending on available resources.

**FIRST PART:**

- Building molecules in space using compact or exploded representation with a molecular model or, if not available, drawing molecules in 3D using software.

Methods for purification of organic materials:

- Mechanical separation methods (filtration, decantation, vacuum filtration, etc.)
- Liquid-liquid extraction
- Refractometry
- Preparation of soap
- Recrystallization of an organic product (benzoic acid or another product).
- Separation of a benzene-toluene mixture by fractional distillation

**SECOND PART: Synthesis of organic compounds**

- Preparation of ethyl bromide; Preparation of methyl iodide
- Preparation of phenetole  $C_6H_5OC_2H_5$  from ethyl bromide and phenol
- Synthesis of aspirin (acetylsalicylic acid)
- Preparation of benzoic acid from toluene
- Synthesis of ortho and para-nitrophenol
- Synthesis of nitrobenzene
- Synthesis of aniline
- Synthesis of phenol from aniline
- Synthesis of anisole  $C_6H_5OCH_3$
- Synthesis of helianthin (methyl orange)
- Synthesis of benzophenone
- Synthesis of ethyl acetate.

- **Bibliographic references**

- J. MADDALUNO, V. BELLOSTA, I. CHATAIGNER, F. COUTY, *Chimie organique, Tout le cours en fiches*, Ed. Dunod, (2013)
- N. L. GERMAIN, J. UZIEL, R. GIL, *Synthèses en chimie organique Exercices corrigés*, Ed. Dunod (2012).

**Semester: 3**

**UE: Fundamental**

**Course: Numerical Methods and Programming**

**Course: Content:**

**Chapter 1. Introduction (or review) of computer programming languages**

MATLAB and/or MATHEMATICA and/or FORTRAN and/or C++,

**Chapter 2. Numerical integration**

2.1 Trapezoidal rule

2.2 Simpson's rule

**Chapter 3. Numerical solutions of nonlinear equations**

3.1 Bisection method

3.2 Newton's method

**Chapter 4. Numerical solutions of ordinary differential equations**

4.1 Euler's method

4.2 Runge-Kutta method

**Chapter 5. Numerical solutions of linear equations systems**

5.1 Gauss elimination method

5.2 Gauss-Seidel method

### **Bibliographic references**

#### **MATLAB**

- M. DJEBLI & H. DJELOUAH, *Initiation à MATLAB*, OPU, (2013).
- R. DUKKIPATI, *MATLAB, an introduction with applications*, New Age International Publishers, India, (2010).
- C. WOODFORD and C. Phillips, *Numerical methods with worked examples: MATLAB edition*, 2<sup>nd</sup> Ed. Springer Ltd, (2013).

#### **C et C++**

- C. DELANNOY, *"C++ pour les programmeurs C"*, 6<sup>ème</sup> Ed., Eyrolles, Paris, (2004).
- C. CASTEYDE, *"Cours de C/C++"*, Copyright, (2005).

#### **FORTRAN**

- B. HAHN, *'Introduction to Fortran 90 for scientists and engineers'*, Capetown University, South Africa, (1993).
- Ph. D'Anfray, *"Fortran 77"*, Université Paris XIII, (1998).
- P. CORDE et A. FOUILLOUX, *Langage Fortran, Support de cours*, IDRIS, (2010).

#### **For numerical methods**

- F. JEDRZEJEWSKI, *Introduction aux méthodes numériques*, 2<sup>ème</sup> Ed., Springer, France, (2005).
- J. HOFFMAN, *Numerical methods for engineers and scientists*, 2<sup>nd</sup> Ed, Marcel Dekker, USA, (2001).
- A. QUARTERONI, *Méthodes numériques, algorithmes, analyse et appl.*, Springer, Italie,



(2004).

**Semester: 3**

**TU discovery**

**Course: Techniques of Physico-Chemical Analysis I**

**Course Content:**

**1. Generalities on separation methods**

Separation of components from a heterogeneous mixture

- Case of a solid-liquid mixture (filtration, centrifugation)

- Case of a mixture of two immiscible liquids

Treatment of a homogeneous phase

**2. Phase separation**

Case of a liquid solution, elimination, relargage

1- Osmosis & dialysis

**4. Chemical extraction**

**5. Extraction by a non-miscible solvent**

Generalities, expression of partition, partition coefficient, distribution rate, expression of yield

Simple extraction: definition, quantitative study, practical implementation of an extraction

**6. Separation by change of state**

Reminder of general concepts, sublimation, simple distillation, rectification (fractional distillation), distillation of a mixture of non-miscible liquids

**7. Chromatographic methods**

Generalities, general principles of chromatography (classification), schematic representation of a chromatogram, theoretical study of chromatography: theory of plateaus, symmetry of peaks, adsorption phenomena, kinetic theory (H.E.P.T. equation of Van Deemter).

Implementation of chromatographic methods: TLC, HPLC, GC, etc.

**8- Electrophoretic methods**

**Bibliographic references**

- G. MAHUZIER, M. HAMON, *Abrégé de chimie analytique : Méthodes de séparation, tome2* ; Ed. Masson, Paris, New York, Barcelone, Milan, (1978).
- M.CHAVANE ; G.J. BEAUDOIN A. JULLIEN; E. FLAMMAND, *Chimie organique expérimentale*, Modulo Editeur, (1986).
- G.GUICHON, C. POMMIER, *La chromatographie en phase gazeuse*, Ed. Gauthier-Villars(1971).
- J. TRANCHANT, *Manuelpratique de chromatographie en phase gazeuse* ; 3<sup>ème</sup> Ed.MASSON ; Paris, New York, Barcelone, Milan, (1982).

**Semester: 3**  
**TU Transversal**  
**Course: Foreign Languages 3**

**Course Content:**

Oral and written expression, communication, and methodology in foreign languages. Training in the understanding of written documents related to the field of physics. We will try to associate language teaching with scientific education as much as possible. All materials will be used, including translation of notices and publications, writing summaries, bibliographies, and project presentations.

**Semestre : 4**  
**TE fundamental**  
**Course: Organic Chemistry 2**

**Course Content:**

**Chapter 1:**

1.1 Physical properties of organic molecules,  
Polarization and dipole moments,  
Polarizability.

**Chapter 2: Electronic effects:**

Inductive effect,  
Mesomeric effect,  
Electromeric effect,  
Conjugation and hyperconjugation.

**Chapter 3: Resonance and Aromaticity.**

**Chapter 4: Classification and study of reactions:**

Homolytic and heterolytic reactions.  
Reaction intermediates.

**Chapter 5: Reaction mechanisms.**

Nucleophilic substitution: SN2, SN1, SNi.  
Elimination: E1, E2 (cis and trans elimination).  
Addition: A1, A2 (cis and trans addition).  
Electrophilic substitution.  
Radical reactions.  
Examples of transposition reactions: Wagner-Meerwein, pinacol, Beckmann.

**Chapter 6: Alkanes, cycloalkanes, alkenes, alkynes.**

**Chapter 7: Arenes.**

**Chapter 8: Halogenated and organomagnesium derivatives.**

**Chapter 9: Alcohols, phenols, ethers.**

**Chapter 10: Amines.**

**Chapter 11: Aldehydes, ketones, carboxylic acids.**

**Chapter 12: Organometallics.**

**Bibliographic references**

- P. ARNAUD. *Cours : Chimie organique*, 18<sup>ème</sup> édition, Dunod, (2009).
- P. ARNAUD. *Exercices de chimie organique*, 4<sup>ème</sup> édition, Dunod, (2010).
- K.P.C. VOLLHARDT, N. E. SCHORE, C. ESKENAZI. *Traité de chimie organique*, 5<sup>ème</sup> édition. De Boeck - Université, (2009).
- J. McMURRY, E. SIMANEK. *Chimie organique Les grands principes : cours et exercices corrigés*. 2<sup>ème</sup> édition, DUNOD, (2007).

**Semestre : 4**

**TU fundamental**

**Course: Thermodynamics and Chemical Kinetics**

**Course Content:**

**THERMODYNAMIC PART**

**Chapitre I :** Thermodynamics of open systems: Characteristic functions of open systems, Notion of chemical potential, Application to chemical reactions.

**Chapitre II :** Chemical equilibria: Homogeneous equilibria, Heterogeneous equilibria.

**Chapitre III :** The pure substance: The pure substance under one phase: The ideal gas ( $\Delta H$ ,  $\Delta S$ , and  $\Delta G$  of the ideal gas), The real gas (Free enthalpy and notion of fugacity), Deviation from the ideal gas, Treatment of some equations of state (Van Der Waals equation, Viriel equation), The pure substance in the condensed state ( $\Delta H$ ,  $\Delta S$ , and  $\Delta G$ ), The pure substance under several phases, General laws of equilibrium (Clapeyron's law, Clausius-Clapeyron's law), Phase rule, Vaporization, sublimation, fusion, and transition of the pure substance.

**Chapitre IV :** Solutions: Solutions under one phase, Partial molar quantities, mixing quantities, Ideal solutions, Real solutions, activity, excess quantities, and mixing quantities. Solutions under several phases, Liquid-vapor equilibrium diagrams; Liquid-solid equilibrium diagrams.

**CHEMICAL KINETIC PART**

**I- Homogeneous Chemical Reactions**

**Chapitre 1-** Reaction rate: Measurement, expressions, experimental, molecular order, composite reactions, temperature influence.

**Chapitre 2-** Simple order reactions: Determination of the global order and partial orders, integration method, differential method, isolation method, order as a function of time and initial concentrations.

**Chapitre 3** Composite reactions: Opposed (inverse), parallel, and successive

reactions, complex reactions, combinations of composite reactions, Complex reactions with steady state of intermediate compounds, reactions in stages, chain reactions.

**Chapitre 4** Elementary act theory: collision theory, pseudo-monomolecular reaction, activated complex theory, activation energy, its measurement; photochemical activation.

## **II- Heterogeneous Chemical Reactions**

**Chapitre 5.** Heterogeneous catalysis: Physical adsorption and chemisorption, physicochemical studies of catalysts, action mechanisms, catalytic kinetics; temperature influence.

**Chapitre 6** Heterogeneous reactions: Study methods, Nucleation law, Diffusion phenomenon, Kinetics of a second-order reaction, Kinetics of a polarimetry reaction, determination of activation energy, Physical characterization of catalysts by adsorption, Solute adsorption on a solid, Reaction kinetics.

### **Bibliographic references**

- M. CHABANEL et B. ILLIEN, *Thermodynamique chimique*, Ed. Ellipses, Paris, (2011).
- J. M. SMITH, H. C. van NESS, A. M. ABBOTT, *Introduction to chemical Engineering thermodynamics*, 2<sup>nd</sup> ed., McGraw-Hill, (1989).
- A. GRUGER, *Thermodynamique et équilibres chimiques, Cours et exercices corrigés*, 2<sup>nd</sup> éd., Dunod, (2004).
- P.L. FABRE, *Thermodynamique et Cinétique Chimique, Résumés de cours et exercices corrigés*, Ed. Ellipses, Technosup, (1998).
- R. MAUDUIT, *Thermodynamique en 20 fiches*, Ed. Dunod, (2013)
- J-C. DECHAUX, L. DELFOSSE, A. PERCHE, *Problèmes de cinétique chimique*, Ed. Masson & Colin, Inter éditions, (1980).
- B. FREMAUX, *Éléments de cinétique et de catalyse*, Éd. Tec. & Doc, (1989).
- G. SCACCHI, M. BOUCHY, J.-F. FOUCAUT, O. ZAHRAA, *Cinétique et Catalyse*, Ed. Tec & Doc., (1996)

**Semestre : 4**

**TU fundamental**

**Course: Analytical Chemistry**

**Course Content:**

**Chapter 1. Equilibria in solution:**

1.1. Homogeneous and heterogeneous equilibria.

The equilibrium constant.

The equilibrium factors.

Le Chatelier's principle.

**Chapter 2. Redox reactions:**

The concepts of redox and reduction.

Oxidation number of an element.

Determination of coefficients of redox reactions.

**Chapter 3. Ionic solutions. Acids and Bases:**

Ionic dissociation (dissociation equilibrium, auto-ionization of water).

Water ion product.

Generalities on acids and bases (definitions, consequences of the Bronsted definition).

Strengths of acids and bases.

**Chapter 4. pH of acids and bases:**

The concept of pH.

Calculation of pH of an acid or a base.

Measurement of pH. Neutralization of an acid by a base.

**Chapter 5. Salts in solution:**

Study of sparingly soluble salts (definitions, solubility of salts, solubility products).

Displacement of solubility equilibrium.

### **Bibliographic references**

- J. L. BRISSET, A. ADDOU, M. DRAOUI, D. MOUSSA, F. ABDELMALEK, *Chimie analytique en solution* (2<sup>ème</sup> Ed.) : Principes et Applications, Lavoisier, (2011).
- J.-L. BURGOT, *Chimie analytique et équilibres ioniques*, (2<sup>ème</sup> Ed.), Lavoisier, (2011).
- C. H. TROTTMANN, M. GUERNET, *Exercices de chimie analytique avec rappels de cours*, Ed. Dunod, Paris, (2011)
- J. W. HILL, R. H. PETRUCCI, *Chimie des Solutions*, Ed. Erpi, (2008)
- P. L. FABRE, *Chimie des Solutions, Résumés de cours et exercices*

**Semestre : 4**

**TU fundamental**

**Course: Quantum Chemistry**

**Course Content:**

**Chapter 1:** General Principles of Quantum Mechanics. 9 hours

Introduction to the basic ideas of quantum theory. Quantum state: wave function. Observable properties and quantum operators. Time evolution of a quantum system: time-dependent Schrödinger equation, conservative energy system, time-independent Schrödinger equation, ground state and excited states. Measuring a property and average value. Uncertainty principle.

**Chapter 2:** Free Particle Model in a Box. 6 hours

One-dimensional potential well. Two- and three-dimensional potential wells. Application: modeling the structure of  $\pi$  electrons in polyenes.

**Chapter 3:** Hydrogen-like Atoms. 9 hours

Hamiltonian, time-dependent and time-independent Schrödinger equations. Solving the Schrödinger equation. Analysis and interpretation of solutions. Introduction of spin: spin-orbital.

**Chapter 4:** Approximation Methods in Quantum Mechanics. 3 hours

Perturbation method. Variational method.

**Chapter 5:** Multi-electron Atoms. 9 hours

Hamiltonian and Schrödinger equation. Orbital approximation. Pauli principle. Slater model. Electronic structure of atoms.

**Chapter 6:** Diatomic Molecules. 9 hours

The  $H_2^+$  molecular ion, CLOA approximation. Interaction of two identical atomic orbitals: homonuclear diatomic molecules. Interaction of two different atomic orbitals: heteronuclear diatomic molecules.

**Bibliographic references**

- B. VIDAL, *Chimie Quantique*, Ed. Masson, (1992).
- D. Mac QUARRIE, J. D. SIMON, *Chimie physique: approche moléculaire*, Ed. Dunod, (2000).
- P. HIBERTY, N. T. ANH, *Introduction à la chimie quantique*, Ed. Ecole Polytechnique, (2008)
- C. LEFORESTIER, *Introduction à la chimie quantique, Cours et exercices corrigés*, Ed. Dunod, (2005).

**Semestre : 4**

**TU Methodology**

**Course: Practical work in Analytical Chemistry**

**Course Content:**

The practical work should focus on acid-base titrations, oxidation-reduction reactions, and precipitation. They can be organized as follows:

1- Preparation of solutions

2- Volumetric analysis and acid-base reactions: Acid-base titrations

- Titration of a strong base with a weak acid (example: NaOH-HCl)
- Titration of a weak acid with a strong base (example: CH<sub>3</sub>COOH with NaOH)
- Double titration of a solution (2 equivalence points) (example: Na<sub>2</sub>CO<sub>3</sub>)

3- Experimental determination of solubility (example: NaCl)

4- Volumetric analysis by oxidation-reduction

- Titration of ferrous ions with permanganate ions
- Titration of an I<sub>2</sub> solution with sodium thiosulfate.

**Bibliographic references**

- J. L. BRISSET, A. ADDOU, M. DRAOUI, D. MOUSSA, F. ABDELMALEK, *Chimie analytique en solution* (2ème Ed.) : Principes et Applications, Lavoisier, (2011).
- J.-L. BURGOT, *Chimie analytique et équilibres ioniques*, (2ème Ed.), Lavoisier, (2011).
- J. W. HILL, R. H. PETRUCCI, *Chimie des Solutions*, Ed. Erpi, (2008)
- P. L. FABRE, *Chimie des Solutions, Résumés de cours et exercices corrigés*, Ed. Ellipses, (2010)

**Semestre : 4**

**TU Methodology**

**Course: Thermodynamics and Chemical Kinetics Lab Work**

**Course Content:**

**Part 1: Thermodynamics Lab Work (Choose 3 labs)**

1. Liquid-vapor Equilibrium
2. Colligative Properties: Determination of Molar Mass by Cryoscopy
3. Determination of Partial Molar Volumes by Pycnometer
4. Measurement of Molar Volume of Mixtures
5. Measurement of Excess Molar Volume
6. Measurement of Heat of Mixing
7. Measurement of Excess Heat

**Part 2: Chemical Kinetics Lab Work (Choose 3 labs)**

1. Kinetics of the Hydration Reaction of Ethyl Acetate
2. Determination of Reaction Rate (2nd Order)
3. Adsorption of a Solute onto a Solid
4. Study of the Persulfate-Iodide Reaction
5. Kinetic Study of the Saponification of Ethyl Acetate by Conductometry
6. Determination of Activation Energy
7. Hydrolysis of Sucrose

**Bibliographic references**

- M. CHABANEL et B. ILLIEN, *Thermodynamique chimique*, Ed. Ellipses, Paris, (2011).
- J. M. SMITH, H. C. van NESS, A. M. ABBOTT, *Introduction to chemical Engineering thermodynamics*, 2<sup>nd</sup> ed., McGraw-Hill, (1989).
- R. MAUDUIT, *Thermodynamique en 20 fiches*, Ed. Dunod, (2013)
- B. FREMAUX, *Éléments de cinétique et de catalyse*, Éd. Tec. & Doc, (1989).
- G. SCACCHI, M. BOUCHY, J.-F. FOUCAUT, O. ZAHRAA, *Cinétique et Catalyse*, Ed. Tec & Doc., (1996)



**Semestre : 4**

**TU Methodology**

**Course: Inorganic Chemistry**

**Course Content:**

**Chapter 1:** Structure of solid materials: General concepts: Amorphous/crystalline state, poly/monocrystals, perfect/real crystal (defects, grain boundaries, surface...). Structure of metallic frameworks. Metallic bonding: band model. Application to the conductivity of metals and semiconductors. Alloys. Structure of atomic and molecular frameworks. Structure and geometry of ionic frameworks. Model of ionic bonding. Lattice energy (solid solutions: insertion, substitution. Real crystal and defects: electronic defects, point defects, linear defects, and planar defects).

**Chapter 2:** Chemistry of transition elements: Coordination complex structures. Optical and magnetic properties. Crystal field theory and molecular orbital theory. Reactivity of complexes. Organometallic compounds.

**Chapter 3:** Introduction to crystallography: Lattice concept. Crystal networks. Multiplicity of a lattice. Rows. Reticular planes. The seven crystal systems. The fourteen Bravais lattices. Symmetry in crystals. Reciprocal lattices of non-primitive lattices.

**Chapter 4:** Metallic structures: Lattice concept. Square arrangement: Semi-compact cubic centered structure CC. Triangular arrangement: Hexagonal close-packed symmetry HC, Cubic face-centered symmetry CFC. Interstitial sites: in CC, in HC, in CFC.

**Chapter 5:** Ionic structures: AB type structures: CsCl, NaCl, ZnS blende, ZnS wurtzite. AB<sub>2</sub> type structure: Fluorine CaF<sub>2</sub>, Rutile TiO<sub>2</sub>

**Chapter 6:** Covalent structures.

#### **Bibliographic references**

- M. SHRAVER, ATKINS, EARSON, *Mass spectrometry*, Ed. J. Wiley, (1992).
- R. KEITER, J. HUHEEY, E. KEITER, *Chimie Inorganique*, Ed. De Boeck, (2000).
- J.-F. LAMBERT, T. GEORGELIN, M. JABER, *Mini manuel de Chimie inorganique*, Ed. Dunod, (2014)
- L. LOPES, *Chimie générale et inorganique, 86 exercices corrigés*, Ed. Ellipses, (2014).

**Semestre : 4**

**TU discovery**

**Course: Techniques of Physicochemical Analysis II**

**Course Content:**

**Chapter 1.** Introduction to spectral methods: definition and generalities on electromagnetic spectra.

**Chapter 2.** Absorption laws and application of the Beer-Lambert law to UV-Visible spectrophotometry: principle. Different absorption domains. Different chromophores. Application in quantitative analysis.

**Chapter 3.** Atomic absorption spectrophotometry: principle and theory. Instrumentation. Characteristics of a flame. Atomization furnace. Interferences. Applications.

**Chapter 4.** Infrared spectrometry: Presentation of the mid-infrared spectrum. Origin of absorptions in the mid-infrared. Vibration-rotation bands of mid-infrared. Simplified model of vibrational interactions. Characteristic bands of organic compounds. Instrumentation. Comparison of spectra.

**Chapter 5.** Nuclear Magnetic Resonance Spectroscopy: Generalities. Spin/magnetic field interaction for a nucleus. Nuclei that can be studied by NMR. Bloch theory for a nucleus with  $I=1/2$ . Principle of obtaining the spectrum by NMR. Hydrogen NMR. Chemical shift. Shielded and unshielded nuclei. Hyperfine structure. Spin-spin coupling.

**Chapter 6.** Mass spectrometry: Principle of the method. Deviation of ions – Bainbridge spectrum. Performance of mass spectrometers. Different analyzers.

**Bibliographic references**

- M. PINTA, *Spectrométrie d'absorption atomique*, Tomes I et II, Ed. Masson, (1979).
- R. DAVIS, M. FREARSON, *Mass spectrometry*, Ed. J. Wiley, (1992).
- B.C. SMITH, *Fundamentals of Fourier Transformed Infrared*, C.R.C Press Inc. (1996).
- E. CONSTANTIN, *Spectrométrie de masse, principe et application*, Ed. Tec-Doc, 2<sup>ème</sup> éd., Paris (1996).
- M. Mc MASTER, *GC / MS Practical User's Guide*, Ed. WILEY- VCH (1998).
- F. ROUESSAC, A. ROUESSAC, *Analyse Chimique. Méthodes et Techniques instrumentales modernes. Cours et exercices résolus*, 5<sup>ème</sup> édition. Dunod, Paris, (2000).

**Semestre : 4**

**TU transversal**

**Course: Foreign Languages 4**

**Course Content:**

- Learning how to write and present a given cultural study.

- Introduction to internet research techniques.

(The goal is to associate language learning with scientific education as much as possible, and all available resources will be used.)

**Semestre : 5**

**TU fundamental**

**Course: Organic Chemistry III**

**Course Content:**

**Chapter 1:** Review of basic concepts in organic chemistry.

- Concept of reaction mechanism.
- Kinetic and thermodynamic aspects of a reaction.
- Electronic aspect.
- Stereochemical aspect.

**Chapter 2:** Reactivity of carbonyls

- General aspects of reactivity, stereochemistry, and activation
- Orbital description
- Action of nucleophiles (other than carbanions)
- Addition reactions: reactivity of aldehydes and ketones towards addition
  - Examples of reactions - Ketenes and isocyanates - Conjugated carbonyl compounds.
- Substitution reactions: substrate and nucleophile reactivity - Examples of reactions.

**Chapter 3:** Enolates

- Kinetics and thermodynamics.
- Alkylation of enolates
- Aldol condensation
- Reactions of enolates with esters and related reactions
- Conjugate additions (or Michael additions).
- Addition of nucleophiles to Michael acceptors.
- Robinson annulation and related reactions.
- Michael additions with enamines.
- Darzens reaction.

**Chapter 4:** Enols

- Halogenation reaction.
- Hell-Volhard-Zelinsky reaction.
- Aldolization.
- Mannich reaction.

**Chapter 5:** Sulfur, phosphorus, and diazomethane compounds

- Thioacetals (polarity inversion of C=O).
- Sulfur ylides.

- Phosphorus ylides.
- Wittig reaction.
- Phosphonates.
- Diazomethane: reaction with ketones and acid chlorides.

**Chapter 6:** Pericyclic reactions (Woodward-Hoffmann rules)

- Electrocyclic reactions.
- Sigmatropic rearrangements: Cope and Claisen transposition.

**Chapter 7:** Oxidation

- Oxidation reactions in organic synthesis.
- Reduction reactions in organic synthesis.
- Protecting groups.
- Multi-step syntheses.

**Bibliographic references**

- P. ARNAUD. *Cours : Chimie organique*, 18<sup>ème</sup> éd. Dunod, (2009).
- P. ARNAUD. *Exercices de chimie organique*, 4<sup>ème</sup> éd. Dunod, (2010).
- *Traité de chimie organique : VOLLHARDT ; SCHORE* , Edition : DE BOECK ; 2015 (6<sup>ème</sup> édition)
- *Chimie organique des hétéro éléments* , Nicolas RABASSO, Edition : DE BOECK ; 2014
- J. McMURRY, E. SIMANEK. *Chimie organique Les grands principes -Cours et exercices corrigés*. 2<sup>ème</sup> éd., DUNOD, (2007).

**Semester 5 :**  
**TU fundamental**  
**Course: Analytical Chemistry II**

**Course Content:**

**Chapter 1:** Basic Statistical Parameters.

- Central value, accuracy, and precision of a set of measurements.
- Variance and standard deviation.
- Random or indeterminate errors.
- Confidence interval of the mean.
- Comparison of results - Parametric tests.
- Rejection test - Q quotient or Dixon's test.
- Calibration curves.
- Robust methods or non-parametric tests.
- Optimization by the one-factor-at-a-time method.

**Chapter 2:** Generalities on Volumetric Titration Methods.

- Definitions of titration methods (volumetry, gravimetry, and coulometry).
- General considerations on titrations (standard substances, standard solutions, solution concentrations, equivalence point, and end point of titration).

**Chapter 3:** pH of Aqueous and Non-Aqueous Solutions.

- Definitions and reminders (acid-base couples,  $K_{aH/A}$ -, solvent R.A.I., operator  $p$ , acid and base strength in relation to the solvent, leveling of acid and base strength by the solvent, Ostwald's dilution law, etc.).
- pH of aqueous and non-aqueous solutions.
- Strong acids: rigorous resolution and discussion of limits of simplified formula use.
- Strong bases: rigorous resolution and discussion of limits of simplified formula use.
- Weak acids (3rd degree equation, simplification to the 2nd degree....).
- $k_a/f$  criterion and average acidity.
- Weak bases and average basicity.
- Buffer solutions: discussion of approximations.
- Amphoteric substances: general resolution.
- Mixtures of acid-base species.
- Acid-base titrations.
- Selection of colored indicators.

**Chapter 4:** Precipitation Titration.

- Titration of halide ions by the Mohr method.
- Titration of halide ions by the Volhard method.
- Chemical indicators during precipitation titrations.

**Chapter 5:** Redox Titration.

- Practical realization.
- Examples of redox titration curves.

- Effect of variables on redox titration curves.
- Redox indicators.

**Chapter 6:** Complexometric Titration.

- Practical realization.
- Complexometric indicators.

**Chapter 7:** Gravimetry.

- Precipitation methods.
- Volatilization methods.
- Gravimetric factor.
- Properties of precipitates and precipitation reagents.
- Mechanisms of precipitate formation.
- Treatment of colloidal precipitates.
- Drying and calcination.
- Organic precipitation reagents.

**Bibliographic references**

1. Exercices de Chimie analytique - Avec rappels de cours - 3e éd : Christine Herrenknecht-Trottmann et Michel Guernet. Edition DONUD ; 2011.
2. Chimie analytique : Chimie des solutions : Martine Beljean-Leymarie et Jean-Pierre Dubost. Edition Masson ; 2006
3. CHIMIE ANALYTIQUE. Tome 2, Méthodes de séparation, 3ème édition : Danielle Ferrer et Michel Hamon. Edition Masson.
4. Chimie analytique et équilibres ioniques : Jean-Louis Burgot. Edition Lavoisier.

**Semestre : 5**

**TU fundamental**

**Course: Crystallography**

**Course Content:**

**Chapter 1: Geometric Crystallography**

1. Orientation symmetry:

- Symmetry element
- Group laws
- Point groups and representation
- Applications

2. Position symmetry:

- Symmetry element
- Translation groups (2D and 3D spaces)
- Molecular symmetry and crystal symmetry
- Space groups and representations
- Applications

3. Reciprocal lattice:

- Direct lattice and reciprocal lattice
- Definitions and properties

**Chapter 2: X-ray diffraction**

1. X-ray radiation and its properties:

- Absorption
- X-ray fluorescence
- Elastic and inelastic scattering

2. X-ray diffraction:

- Symmetry elements and diffraction
- Scattering factor
- Structure factor
- Ewald sphere
- Diffraction and reciprocal lattice

**Chapter 3: Radiocrystallography methods**

1. Powder method

2. Single crystal methods



## **Bibliographic references**

- [1] Jean-J. Rousseau « Cristallographie géométrique et radiocristallographie : Cours et exercices corrigés - Licence 3, Master », Dunod, 3e édition , 2007.
- [2] D. Rioux « Introduction à la cristallographie. Solide cristallisé et empilements compacts », Ellipses, 2007.
- [3] D. Schwarzenbach et G. Chapuis « Cristallographie », Presses Polytechniques et universitaires Romandes (PPUR), 2006.
- [4] F. Mathieu « Exercices et problèmes de cristallographie », Cépaduès, 2002.

**Semestre : 5**

**TU fundamental**

**Course: Quantum Chemistry II**

**Course Content:**

**Chapter 1:** Basic approximations.

- Writing the Hamiltonian of a molecule
- Separation of nuclear and electronic motions: Born-Oppenheimer approximation
- Separation of electronic motions: orbital approximation
- LCAO method

**Chapter 2:** Molecular electronic structure: Qualitative approach.

- Interaction of two identical atomic orbitals: homonuclear diatomic molecules
- Interaction of two different atomic orbitals: heteronuclear diatomic molecules
- Interaction of three orbitals: AH molecules
- Interaction of four orbitals: A<sub>2</sub> molecules
- Interaction of four orbitals: AB molecules
- Electronic properties of diatomic molecules (population analysis, Mulliken charge, dipole moment, bond order, etc.)

**Chapter 3:** Molecular electronic structure: Quantitative approach.

- Simple Huckel method (principles and applications)
- Extended Huckel method (principles and applications)

**Chapter 4:** Elements of quantum theory of chemical reactivity.

- Frontier orbitals: definition and identification
- Prediction of reactive sites: nucleophilic and electrophilic attacks, cyclization

**Chapter 5:** Orbital interactions in organometallic complexes.

- Eighteen-electron rule
- M<sub>L</sub>*n* complexes (M<sub>L</sub>6, M<sub>L</sub>5, etc.)

**Bibliographic references**

1. Introduction à la chimie quantique : Claude Leforestier. Edition Dunod ; 2005.
2. Element de Chimie quantique à l'usage des chimistes (2<sup>e</sup> édition) : Jean-Louis Rivail. Edition : EDP Sciences ; 1999.
3. B. VIDAL, *Chimie Quantique*, Ed. Masson, (1992).
4. D. Mac QUARRIE, J. D. SIMON, *Chimie physique: approche moléculaire*, Ed. Dunod,(2000).
5. P. HIBERTY, N. T. ANH, *Introduction à la chimie quantique*, Ed. Ecole Polytechnique,(2008)
6. C. LEFORESTIER, *Introduction à la chimie quantique, Cours et exercices corrigés*, Ed. Dunod, (2005).

**Semestre : 5**

**TU methodology**

**Course: PW Analytical chemistry**

**Content of the subject:**

1. Errors in chemical analysis: Errors in volume measurements.
2. Potentiometric acid-base titration. Effect of concentrations and acid dissociation constants on titration curves.
3. Potentiometric titration of a weak polyacid with a strong base. Comparison with colorimetric titration.
4. Chloride determination in water (sea water, tap water, and mineral water) by the Mohr method.
5. Complexometric titration: Determination of water hardness (tap water, spring water, and mineral water).
6. Gravimetric determination of sulfate ions in water.

**Bibliographic references**

1. Travaux pratiques de chimie : De l'expérience à l'interprétation : Thomas Barilero et Aurélie Deleuze. Edition Rue D'ulm ; 2013.
2. J. L. BRISSET, A. ADDOU, M. DRAOUI, D. MOUSSA, F. ABDELMALEK, *Chimie analytique en solution* (2<sup>ème</sup> Ed.) : Principes et Applications, Lavoisier, (2011).
3. J.-L. BURGOT, *Chimie analytique et équilibres ioniques*, (2<sup>ème</sup> Ed.), Lavoisier, (2011).
4. J. W. HILL, R. H. PETRUCCI, *Chimie des Solutions*, Ed. Erpi, (2008)
5. P. L. FABRE, *Chimie des Solutions, Résumés de cours et exercices corrigés*, Ed. Ellipses, (2010)

**Semestre : 5**  
**TU methodology**  
**Course: PW Molecular modeling**

**Course Content:**

- 1- Introduction to the use of a molecular modeling software with a graphical interface.
- 2- Representation, visualization and creation of 2D and 3D molecular structures.
- 3- Performing electronic structure calculations of a molecule using the simple Huckel method.
- 4- Performing electronic structure calculations of a molecule using the extended Huckel method.
- 5- Determination of reactivity indices.

**Bibliographic references**

- [1] M.Rappaz, M. Deville et M. Bellet « Modélisation Numérique en science des matériaux » PPUR presses polytechniques, 1998.
- [2] M. Brissaud, « Matériaux piézoélectriques : caractérisation, modélisation et vibration », PPUR presses polytechniques, 2007
- [3] F.Radjai « Modélisation numérique discrète des matériaux granulaires », Hermes science publications, 2010.
- [4] La modélisation moléculaire à la découverte des composés bioactifs : Dragos\_Horvath. Editions Universitaires Europeennes ; 2011

**Semestre : 5**

**TU discovery**

**Course: Environmental Chemistry**

**Course Content:**

I- Environmental study spheres:

I.1- Composition of the Earth

I.2- Interior of the Earth

I.3- Structure of the atmosphere

I.4- Hydrosphere water cycle

II- Global cycles of elements:

II.1- Oxygen cycle

II.2- Nitrogen cycle

II.3- Carbon cycle

III- Atmospheric pollution:

III.1- Atmospheric properties

III.2- Urban compounds

III.3- Pollutants in the troposphere

III.3.1- Anthropogenic emissions and their sources

III.3.2- Natural emissions and their sources

III.3.3- Case of CO<sub>2</sub> and methane

III.3.4- Presence of rain

III.3.5- Physicochemical transformations of pollutants in the atmosphere

III.4- Stratosphere

III.4.1- Generalities

III.4.2- Stratospheric ozone cycle

III.4.3- Disturbance of the Chapman cycle

- By natural gases

- By CFCs

IV- Soil pollution:

IV.1- Generalities

IV.2- Polluting substances in the soil

IV.3- Sources of pollution

IV.4- Behavior of pollutants in the soil

IV.5- Heavy metals

V- Water pollution:

V.1- Natural waters

V.2- Water pollutants

V.3- Water analysis

**Bibliographic references**

[1]. Chimie de l'environnement : Claus Bliefert, Robert Perraud. Edition De Boeck ; 2008.

**Semestre : 5**  
**TU transversal**  
**Course: Scientific English I**

**Course Content:**

- General introduction.
- English text structure.
- General chemistry glossary.
- Laboratory description.
- Scientific Experiment description.
- Write a scientific experiment resume.
- Materials classes' description and scientific references.
- Materials science and engineering key words.

**Bibliographic references**

- [1] Robert A. Day « Scientific English: A Guide for Scientists and Other Professional », Oryx Press, 1995
- [2] Jack P. Hailman, Karen B. Strier « Planning, Proposing and Presenting Science Effectively: A Guide for Graduate Students and Researchers in the Behavioral Sciences and Biology », Cambridge University Press, 2006
- [3] Robert A. Day, Nancy Sakaduski, Nancy Day «Scientific English: A Guide for Scientists and Other Professionals», Third Edition, ABC-CLIO, 2011
- [4] Write away , Rédiger en anglais scientifique et technique : Jocelyne Boulon, Hervé Marchand. Edition Ellipses ; 2012.

**Semestre : 6**

**TU fundamental**

**Course: Thermodynamics of solutions**

**Course Content:**

**Chapter 1: Chemical Potential**

- Definition.
- Chemical Potential of a Pure Substance.

**Chapter 2: Partial Molar Properties (PMP)**

- Properties of PMP.
- Determination of PMP.
- Mixing Properties.

**Chapter 3: Fugacity of Real Gases**

- Definition.
- Determination of Fugacity (variation with Pressure, fugacity in Reduced Coordinates, Fugacity and Mass Action Law, variation with Temperature).

**Chapter 4: Activity of Molecular Solutions**

- Definition.
- Ideal Solutions (definition, properties of ideal solutions).
- Excess Properties (definition, variation of excess properties, empirical expressions of excess properties, classification of solutions by excess properties).
- Empirical Models (Vanlaar, Margules, and Redlich-Kister).
- Semi-Empirical Models (NRTL and Wilson).
- Group Contribution Models (DISQUAC, UNIFAC).
- Regular Solution Model.
- Athermal Solution Model.

**Chapter 5: Critical Phenomena and Liquid-Liquid Equilibrium Diagrams**

- Critical Phenomena.
- Liquid-Liquid Equilibrium Diagrams of Binary Systems.
- Liquid-Liquid Equilibrium Diagrams of Ternary Systems.

## Bibliographic references

- M. CHABANEL et B. ILLIEN, *Thermodynamique chimique*, Ed. Ellipses, Paris, (2011).
- J. M. SMITH, H. C. van NESS, A. M. ABBOTT, *Introduction to chemical Engineering thermodynamics*, 2<sup>nd</sup> ed., McGraw-Hill, (1989).
- A. GRUGER, *Thermodynamique et équilibres chimiques, Cours et exercices corrigés*, 2<sup>nd</sup> éd., Dunod, (2004).
- P.L. FABRE, *Thermodynamique et Cinétique Chimique, Résumés de cours et exercices corrigés*, Ed. Ellipses, Technosup, (1998).
- R. MAUDUIT, *Thermodynamique en 20 fiches*, Ed. Dunod, (2013)
- Thermodynamique chimique - Etats de la matière, équilibres, gaz, solutions, ions : Martial Chabanel, Bertrand Illien. Edition Ellipses ; 2011.
- Thermodynamique PTSI : Georges Faverjon. Editeur(s) : Bréal ; 2003.
- L'indispensable en thermodynamique chimique - Les applications : Jean- Claude Legrand. Edition Bréal ; 2004.



**Semestre : 6**

**TU fundamental**

**Course: Electrochemistry**

**Course Content:**

**Chapter 1: Current Conduction**

- Electric conductors and electrolytic conductors.
- Electrolysis and electrolyte.
- Faraday's Law.
- Activity of electrolytes.

**Chapter 2: Ion Conductivity**

- Ion velocity.
- Current density through the electrolytic cell.
- Conductivity, Equivalent conductivity.
- Transport number.
- Application of conductometry.

**Chapter 3: Electrode Potential**

- General overview.
- Nernst equation, electrode potential.
- Generalized Nernst equation.
- Different types of electrodes.
- Voltage scale.

**Chapter 4: Electrochemical Cells**

- Electromotive forces.
- Examples of cells.
- Cells and thermodynamic properties.
- Applications.

**Bibliographic references**

- [1] C.Lefrou, P. Fabry et J-C. Poignet « L'électrochimie. Fondamentaux avec exercices corrigés », les Ulis- EDP Sciences, DL.2009.
- [2] Fabien Miomandre, Saïd Sadki , Pierre Audebert , Rachel Méallet-Renault « Électrochimie. Des concepts aux applications » , Dunod, 2e édition, 2011.
- [3] C. Montella et J.P diard « Exercices de cinétique électrochimique », Herman, 2000.
- [4] Y. Verchier et F. Lemaître « De l'oxydo- réduction à l'électrochimie », Ellipses, 2006
- [5] L'indispensable en électrochimie : Valérie Bertagna (Auteur), Marius Chemla. Edition Bréal ; 2001.
- [6] L'Électrochimie Concepts fondamentaux illustrés : Christine LEFROU, Pierre FABRY et Jean-Claude POIGNET. Editeur EDP SCIENCES ; 2013.

**Semestre : 6**

**TU fundamental**

**Course: Molecular spectroscopy**

**Course Content:**

**Chapter 1:** Molecular Symmetry and Group Theory.

Elements of molecular symmetry, Matrix representation of symmetry elements, Molecular symmetry groups, Character table of a molecular symmetry group.

**Chapter 2:** Introduction to Molecular Spectroscopy.

Generalities and experimental aspects of absorption spectroscopy.

**Chapter 3:** Rotational Spectroscopy.

The rigid rotor model, Eigenfunctions and eigenenergies, Selection rules, Non-rigid rotor model and centrifugal distortion effects, Rotational spectra of diatomic and polyatomic molecules.

**Chapter 4:** Vibrational Spectroscopy.

The harmonic oscillator model, Eigenfunctions and eigenenergies, Selection rules, Anharmonic oscillator model, Vibrational spectra of diatomic and polyatomic molecules.

**Chapter 5:** Vibrational-Rotational Spectroscopy.

The rotating oscillator model, Vibrational-rotational spectra, Interaction between vibration and rotation, Relationship between molecular constants, Isotopic effect.

**Chapter 6:** Raman Spectroscopy.

Light scattering, Experimental observation of the Raman effect, Theory of the Raman effect, Raman spectra.

**Bibliographic references**

[1] F. Rouessac, A. Rouessac et D. Cruché « Analyse chimique : Méthodes et techniques instrumentales modernes, cours et exercices corrigés », Dunod, 2006.

[2] D. Kiemle « Identification spectrométrique des composés organiques », De Boeck, 2<sup>e</sup> édition, 2007

[3] R. M. Silverstein, G. C. Bassler, T. C. Morrill « Identification spectrométrique des composés organiques », De Boeck, 1998.

[4] D. A. Skoog, F. J. Holler et T. A. Nieman « Principes d'analyse instrumentale », De Boeck, 2003.

[5] Spectroscopie : Cours et exercices : Michael-J Hollas. Edition Donod ; 2003.

**Semestre : 6**

**TU fundamental**

**Course: Surface chemistry and catalysis**

**Course Content:**

**Part: Surface Chemistry and Catalysis**

**Part: Surface Chemistry**

**Chapter 1: Adsorption**

- Gas-phase adsorption (Monolayer adsorption: Freundlich isotherm, Langmuir isotherm / Multilayer adsorption: BET isotherm, different isotherm curves / Specific surface area, porosity, measurement techniques).
- Liquid-phase adsorption (Gibbs model).

**Chapter 2: Surface Tension**

- Concept of surface tension.
- Surface tension and chemical reaction.

**Part: Catalysis**

**Chapter 1: Homogeneous Catalysis**

- Michaelis model.
- Example of enzymatic catalysis.

**Chapter 2: Heterogeneous Catalysis**

- Physisorption, chemisorption.
- Heterogeneous catalysis kinetics (Langmuir-Hinshelwood model, Eley-Rideal model).

**Chapter 3: Practical aspects in catalysis**

- Catalyst supports: aluminas, silica, USY zeolites, activated carbons...
- Support shaping.
- Main catalyst manufacturing operations.

**Chapter 4: Main physical techniques for catalyst characterization.**

**Bibliographic references**

- [1] Gabor A. Somorjai, Delplancke « Chimie des surfaces et catalyse », Techniques industrielles et sciences de l'ingénieur, Ediscience, 2002.
- [2] Dieter Landolt « Corrosion et chimie de surfaces des métaux » *Volume 12 de Traité des matériaux*, PPUR presses polytechniques, 1997
- [3] Robert Lévêque « Traitements et revêtements de surface des métaux », Dunod, 2013.
- [4] Hans Jörg Mathieu, Erich Bergmann « Traité des matériaux, tome 4 : Analyse et technologies des surfaces : Couches minces et tribologie », Presses Polytechniques et Universitaires Romandes (PPUR), 2003.

**Semestre : 6**

**TU methodology**

**Course: Practical work in Electrochemistry**

**Course Content:**

- Conductivity of electrolytes and conductimetric titration
- Determination of the pH of different types of solutions
- Electrolysis. Verification of Faraday's law
- Preparation and study of a second species electrode
- Electrolytic preparation of Sodium Hypochlorite or "Bleach" 6- Determination of the standard potential of an electrode

**Bibliographic references**

[1] Méthodes électrochimiques d'analyse : Jean-Louis Burgot. Edition Lavoisier 2012

**Semestre : 6**

**TU methodology**

**Course: Practical work Physico-chemical methods**

**Course Content:**

- Identification of functional groups
- Thin-layer chromatography
- Characterization by UV and IR spectroscopies
- Characterization by powder X-ray diffraction

**Bibliographic references**

- G.GUICHON, C. POMMIER, *La chromatographie en phase gazeuse*, Ed. Gauthier-Villars (1971).
- J. TRANCHANT, Manuel pratique de chromatographie en phase gazeuse ; 3ème Ed. MASSON ; Paris, New York, Barcelone, Milan, (1982).
- Analyse chimique : Méthodes et techniques instrumentales : Francis Rouessac et Annick Rouessac. Edition Dunod ; 2009.

**Semestre : 6**

**TU discovery**

**Course:Ethics and deontology**

**Course content:**

- Ancient and Modern Deontology:
- The Minimalist Perspective
- Principle of Sobriety
- Principle of Stability
- Principle of Neutrality
- Minimalism and Pluralism

**Bibliographic references**

- [1] M.F Bernier « Ethique et Déontologie », les presses de l'université Laval, 2004
- [2] Québec « code de déontologie des chimistes » chap.C-15, r.4, Québec, 2015
- [3] Législation, éthique, déontologie : Carène Ponte et Alain Broca. Edition : Elsevier Masson ; 2013.

**Semestre : 6**

**TU transversal**

**Course: Ethics and deontology**

**Course content:**

- Reading a scientific paper.
- Introducing a scientific subject.
- Discussing a scientific result.
- Scientific oral communication cases.
- Writing a scientific paper.
- Work group on paper writing.

**Bibliographic references**

- [1] Joshua Schimel Writing Science: How to Write Papers That Get Cited and Proposals That Get Funded, Oxford University Press; 1 edition, 2011
- [2] Paul J. Silvia How to Write a Lot: A Practical Guide to Productive Academic Writing», AmerPsychological Assn; 1 edition, 2007
- [3] Helen Sword « Stylish Academic Writing », Harvard University Press, 2012
- [4] Anglais, prépas scientifiques filières MP, PC, PSI, TSI : Martine Texier-Tolicetti, Briséis Dario. Editeur(s) : Hachette ; 2013