University of Lille

Semester 2 Syllabus

Course catalog	ECTS
Physical Organic Chemistry	5
Structural Inorganic Chemistry	5
Synchrotron Radiation and its Applications	5
Advanced Kinetics	5
Chemometrics	5
Methods in Environmental Chemistry	5
Spectroscopy for Biology	5

Mandatory Courses (first five courses)

Elective courses (5 ECTS to choose) (last two courses)

Physical Organic Chemistry
5 ECTS

Description

This course builds upon the knowledge in organic chemistry previously acquired by the students during Bachelor degree programs (SN1, SN2, E1, E2 and EAS polar reaction mecanisms and radical reactions).

Part 1 - The underlying principles and rationale of organic reactions (Dr Mael Penhoat, 16h)

Physical organic chemistry focuses on understanding the structure, behaviour and reactivity of organic molecules. This part of the course will be divided into three major topics:

- Kinetics & thermodynamics of organic reactions;
- Linear free energy relationships used in the study of reaction mechanisms and in the description of Quantitative Structure Activity Relationships (QSAR): Hammett theory, Taft equation;
- Acid-base catalysis (including Brønsted catalysis equation and plots, kinetic isotope effects)

Part 2 - Orbitalar approach to pericyclic reactions (Dr Cedric Lion, 16h)

Pericyclic reactions are the third important class of organic reactions. They occur via concerted electronic rearrangements of p-systems through the formation of cyclic transition states. Because they allow for fine regio- and stereochemical control, these concerted processes are very popular and have wide applications both in organic and bioorganic chemistry.
After a reminder on molecular orbitals and orbital symmetry, the theoretical concepts allowing for the regiospecificity and diastereospecificity of pericyclic reactions will be covered (Woodward-Hoffman rules, Fukui theory on Frontier Molecular Orbitals, Dewar-Zimmerman models). The three main types of pericyclic reactions will be reviewed:

- Electrocyclic reactions
- Cycloadditions
- Sigmatropic rearrangements and group transfers

Part 3 - Practical sessions (Dr Cedric Lion, 18h)

Besides theoretical lectures and workshops, practical sessions will also be carried out by students in small groups (*Dr Cedric Lion, 24h*). The preparation and purification of various organic molecules in accordance with the lecture program will be followed by their analysis using various spectroscopic techniques (IR, liquid-state NMR, mass spectrometry...). Molecular modeling (calculation of molecular orbitals and product / transition state geometry optimization using *ab*

initio methods) will also be used as a tool for predicting regiospecificity and/or stereospecificity of the undertaken reactions in order to fully apply theory to practice.
Towards the end of the semester, the bibliographic skills of the students will be further developed through an oral presentation on a given topic in conjunction with the lectures.

A final written examination will be performed at the end of the lecture course, and the practicals will be evaluated with a written report.

Aims

The aims of this unit are:

- To develop the skills and confidence of the students in organic chemistry;
- To identify appropriate methodologies for the elucidation of reaction mechanisms and reaction intermediate or product structures (including stereochemical aspects).

Outcomes

After completing this unit the student should be able to:

- Discuss in a comprehensive way the different reaction mechanisms in organic chemistry;
- Identify the most suitable spectroscopic, computational or analytical methodologies for specific applications;
- Evaluate the regio- and stereochemical outcome of polar or pericyclic reactions;
- Give a full interpretation of spectral data, towards the structure elucidation of synthesized or isolated products (including stereochemical aspects);
- Combine all aspects of a given problem in organic chemistry with a critical view: theoretical expectations, practical issues and experimental results obtained through the use of analytical and spectroscopic techniques;
- Present the conclusions drawn in written and oral form, in a clear and concise manner.

Activities

Lectures: 32 hours
Practicals: 18 hours
Student centered learning: 66 hours
Total student effort: 116 hours

Assessment

- Written examination (50%)
- Practical reports (30%)
- Oral presentation (20%)

Advanced Kinetics
5 ECTS

Description

The course covers both the theoretical aspects and the applications of physical chemistry in the field of reactive systems like homogeneous and heterogeneous chemical kinetics and catalysis. Theoretical aspects of chemical kinetics include theories of elementary reactions, approximation methods in chemical kinetics, complex and chain reactions, flame and explosions, gas and condensed phases kinetics. Introduction of principles, theories and concepts of heterogeneous catalysis and the study of catalysis processes is also studied.
The course includes reactors (batch reactor, flow tube, perfect stirred reactor) studies associated with analytical and spectroscopic techniques to study reactive systems in different phases (gas, liquid, solid phases). Kinetics investigations of time dependence of an elementary process cover temperature measurement, classical discharge flow apparatus (associated with detection techniques like resonance fluorescence, laser induced fluorescence, mass spectrometry, laser magnetic resonance), flash photolysis (associated with absorption spectroscopy, fluorescence techniques), shock tubes and relaxation techniques. Kinetic study of more complex reactive systems, like auto-inflammation, flames or clean processes, include coupling of probe and molecular beam sampling with classical analytical methods (GC, GC/MS, FTIR, UV-Vis, …) and laser diagnostics (laser induced fluorescence, Raman spectroscopy, …). Application of in situ spectroscopic techniques for studying catalytic reactions - covering adsorption, kinetic of elementary steps, nature of intermediates- are considered.
Modelling of the reactivity of complex systems is also studied.
Typical applications of particular couplings of the experimental techniques in different areas of physical chemistry -catalysis, engines, flames, aeronautic, atmospheric chemistry, clean processes, environment,… are used as examples.

Aims

- To build upon and extend the theoretical and experimental approaches introduced during the bachelor degree programme.
- To develop the competence and confidence of the students in reaction kinetics and catalysis.
- To identify appropriate experimental procedures for particular application.
- To highlight modern advances in instrumentation and quantitative analytical techniques and their applications.

Outcomes

After completing this unit the student should be able to:

- Discuss in a comprehensive way the methods of sample definition and handling problems encountered in chemical kinetics and catalysis.
- Critically evaluate applicability of a specific experimental technique to study a particular problem in chemical engineering.
- Identify the most suitable instrumentation for specific applications and describe the extent and limitations of the data obtained.
- Interpret the results of an experimental study and present the conclusions in written and oral form.
- Explain to non-specialists how different associated analytical methods can provide valuable information in physical chemistry and environmental sciences.

Activities

Lectures: 30 hours
Practicals: 8 hours
Lab Project: 8 hours
Student centered learning: 26 hours
Total student effort: 72 hours

Examples of Laboratory Project (LP):
LP1: Measurement of NO by FTIR in biofuels flames
LP2: Design of a setup for liquid phase Raman kinetics Studies
LP3: Operando Raman Study of De NOx Catalysts
LP4: Study of soot by Laser Induced Incandescence in biofuels flames
LP5: Species concentration measurements using laser spectroscopic methods in combustion

Practicals works (PW):
PW1 : Kinetics of an autocatalytic reaction (experimental and modeling study)
PW2 : Kinetic study of an isomerisation reaction by flash photolysis

RECOMMENDED READING:
M.J. PILLING, P.W. SEAKINS, Reaction Kinetics, Oxford Science Publications, 1997
J.I. STEINFELD, J.S. FRANCISCO, W.L HASE, Chemical Kinetics and Dynamics , Prentice Hall Inc., 1989
P.W. ATKINS, Physical Chemistry, Oxford University Press, 1990

Assessment

Written Examination: 2/3 of final mark
2 practical work sessions: 1/6 of final mark
1 lab project: 1/6 of final mark

Chemometrics
5 ECTS

Description

In every field of chemistry, data extraction from lab experiments is needed. With computer controlled experimental procedures, chemistry is nowadays an experimental discipline producing an always growing amount of data, up to a point where it is now impossible to analyze spectroscopic data without the appropriate data processing method capable of extracting the wanted information. The proposed course will detail the potential and the limits of different data processing methods in spectroscopy, as an introduction to chemometrics, this new discipline in chemistry.

Course content :

- Data preprocessing algorithms;
- Multivariate regression (MLR, PCR …);
- Classification methods (K-NN, LDA, SIMCA …);
- Multivariate curve resolution methods.

Aims

This course will propose to answer to different aspects such as: qualitative, quantitative analyses, imaging problems, and time resolved spectroscopies data exploration. In conclusion, the aim is to obtain a better understanding of the data processing step for spectroscopic data analysis.

Outcomes

After completing this unit the student should be able to propose different data processing methods in order to extract hidden information from various spectroscopic data.

Activities

Lectures: 18 hours
Practicals: 24 hours
Student centered learning: 84 hours
Total student effort: 126 hours

Assessment

Written examination

Experimental methodologies in environmental sciences
5 ECTS

Aims

- Acquire the basics in environmental chemistry (air, water, soil),
- Acquire the basics in spectroscopy and analysis techniques applied to environmental issues,
- Apply these basics to problems related to environmental issues.

Activities

Lectures and colloquia : 30 hours
Student centered learning : 12 hours
Project : 20 hours

Assessment

Written examination (2 hours)
Project : Oral presentation

Spectroscopy for biology
5 ECTS

Description

The objectives of the unit are to enhance the knowledge in the use and utility of spectroscopic methods in the field of biomolecular analysis.

The course will be divided into three topics dedicated to biomolecular analysis using NMR, SPR and MS. The course will be devoted to the analysis of different classes of biomolecules suitable for these technologies, the strategies to be employed and the type of information (degree of characterization) that they can bring.

The teaching program will cover fundamental and instrumental aspects will focus on different applications and strategies for biomolecular analysis as well as data interpretation. The theoretical learning will be completed by a practical part.

DETAILED CONTENT :

1. Plasmonics: 10H (S. Szunerits)

Objectives: acquire basis knowledge of plasmonic spectroscopy, concept of label-free detection, introduction to surface chemistry, recent developments for miniaturisation of plasmonic transducers

Context: Surface plasmon resonance (SPR) in metals, binding evaluation of targeted analytes using SPR, electrochemical SPR, SPR Fluorescence Spectroscopy, plasmonic properties of metallic particles, formation of metallic nanoparticles in solution and on surfaces, optical wave guides, applications

2. Mass spectrometry: 8H (I. Fournier)

Objectives: complete the formation on MS acquired at S3 by acquiring knowledge on MS of different classes of biomolecules. This includes strategies for biomolecules analysis as well as different identification methods. Focused will be given to peptides/proteins and lipids. The objective is to acquire knowledge on the methods and strategy to be used for each biomolecules class as well as interpretation of data

Context: biomolecules analysis by Mass Spectrometry (MS), analytical MS strategies, identification of biomolecules by MSn, applications in biological studies, quantification of biomolecules, Mass Spectrometry Imaging

3. NMR: 10H (G. Lippens)

Objectives: In-depth description of the HSQC experiment, with notions of solvent suppression. Triple resonance spectroscopy for the assignment of proteins. Interaction mapping by NMR, with the different regimes of exchange. Basics of relaxation theory. Structure calculus by NOE and RDC parameters.

Context: Structural biology – interaction mapping in the context of systems biology and pharmaceutical search of small-molecule interactors.

Aims

- Enlarge the basic knowledge on spectroscopy methods as applied to biomolecular analysis.
- Understand the difference in the divers characterization strategies that can be used and developed for the different classes of biomolecules and identify their specificity.
- Acquire knowledge on data interpretation for biomolecules.
- Learn integrative strategies to answer biological problems using NMR, SPR and MS.

Outcomes

Acquired skills:

- Theoretical knowledge on the strategies, experiments and data interpretation for NMR, MS and SPR of biomolecules
- Identify the methods specificity and level of characterization
- Identify the different strategies to be developed to study biomolecules
- Acquire knowledge on the most recent advances in spectroscopy biomolecules analysis
- Practical knowledge of NMR, MS and SPR analysis of biomolecules

Competencies:

- Ability to know what technique and strategy to use to answer a biological question
- Ability to interpret the data coming out the different strategies

Activities

Lectures: 28 hours
Practicals: 18 hours
Student central learning: 37 hours
Total student effort: 103 hours

Assessment

For the unit evaluation, students will be asked to write a **bibliographic report** on the different techniques they have been taught by showing how do these techniques are complementary and are used together for answering a biological problematic. The report will be completed by an **oral presentation** and followed by questions and discussions with the jury.
Examination of the course period will correspond to a case study given to the students at the beginning of the course. Through literature research and personal input a strategy plan should be built to respond to the given problematic. The students will be asked to present their work as a written report completed by an oral presentation.