Université de Lille

University of Lille

Semester 1 Syllabus

Course catalog	ECTS
Quantum Chemistry and Chemical Bonding	5
Magnetic Resonance	5
Optical Spectroscopy	5
X-ray diffraction	5
Mass Spectrometry	5
English and Professionalisation	5

Mandatory Courses

Quantum Chemistry and Chemical Bonding
5 ECTS

Description

I/ Introduction to quantum mechanics (6 hours)

- The postulates and their application to simple problems: particle in a box, harmonic oscillator;
- Properties of angular momentum: application to the rigid rotor model.

2/ The hydrogen atom (8 hours)

- Solution of the Schrödinger equation: definition of atomic orbitals;
- Properties of the atomic orbitals – energy levels – introduction to atomic spectroscopy;
- Magnetic properties – the spin angular momentum – the spin-orbit coupling – influence on the atomic spectrum.

3/ The two electron problem (6 hours)

- Antisymmetry of the total wavefunction: Slater determinant;
- Perturbation method: introduction of the bielectronic operator – definition of the coulomb and exchange integrals;
- Symmetry and spin properties of the wavefunction: the notion of spectroscopic term;

4/ Polyelectronic systems (6 hours)

- Spectroscopic terms for independent and equivalent electrons;
- Atomic spectroscopy.

5/ Molecular orbitals for diatomic molecules (6 hours)

- The variation method and the molecular orbitals for the H2+ molecular ion;
- Generalization to other diatomic molecules: symmetry properties of the molecular orbitals;
- Spectroscopic terms and electronic spectra.

6/ Molecular orbitals of polyatomic molecules (10 hours)

- Group theory and molecular orbitals;
- Determination of the spectroscopic terms for polyatomic molecules.

7/ Molecular orbitals for transition metal complexes (8 hours)

- Octahedral, tetrahedral and square plane complexes;
- Link between the MO approach and the crystal field approach;
- Introduction to Tanabe-Sugano diagrams.

Aims

The aim of the course is to recall the basic concepts of quantum mechanics and to apply them in the field of electronic structure of atoms and molecules.

Outcomes

After completing the course, the student is able to apply quantum mechanics to various chemistry and spectroscopy related problems.

The student is able to:

- Determine the electronic structure of the ground and excited state of polyelectronic atoms;
- Interpret atomic spectra;
- Build molecular orbitals diagram for polyatomic molecules using character tables;
- Determine the spectroscopic terms for ground and excited states of complex molecules;
- Interpret UV-vis spectra.

Activities

Lectures: 50 hours.
Student centered learning: 50 hours.
Total student effort: 100 hours.

Assessment

2 Written Exams : one on the atomic problem, the other on the molecular problem (2 hours)

Université de Lille

Magnetic Resonance

5 ECTS

Description

This course builds upon the basic notions in magnetic resonance spectroscopy previously acquired by the students at bachelor level.

- The broad impact of magnetic resonance in different fields will be presented, including chemical analysis, material characterization, structural and dynamics investigation of biomolecules medical imaging but also chemical engineering and cultural heritage. The essential concepts of nuclear magnetism and spin dynamics will then be introduced for a good understanding of 1D and 2D routine NMR pulse sequences employed in high-resolution liquid-state NMR (***Pr O. Lafon, 14h***)

- The methods, benefits and limitations of 1D & 2D 1H and 13C NMR will be studied in depth. The influence of the involved physical phenomena on the aspect of NMR spectra will be detailed, with an emphasis on the direct links between the electronic environment of specific nuclei integrated in organic functional groups and their chemical shift. Through-bond and through-space correlations will be reviewed, leading to the use of various homonuclear and heteronuclear 2D NMR experiments (COSY, NOESY, HMQC, HMBC...) towards the structural elucidation of complex bioorganic or synthetic molecules, including stereochemical aspects. (***Dr C. Lion, 22h***)

- The basics of solid-state NMR will be introduced with a special attention towards the Magic Angle Spinning (MAS) technique. Dipolar scalar and quadrupolar interactions will be treated, with a particular focus on advanced methodologies allowing for high resolution and correlation mapping. (***Dr G. Tricot, 8h***)

Aims

The aims of this unit are:

- To show the broad impact of magnetic resonance in chemistry, physics, engineering, biology and medicine;
- To deepen the student's knowledge of NMR and ESR from a theoretical and instrumental point of view;
- To develop the skills and confidence of the students applying various complementary Magnetic Resonance experiments towards structural elucidation;
- To highlight modern advances in instrumentation and techniques within NMR and ESR.

Outcomes

After completing this unit the student should be able to:

- Know for which systems magnetic resonance can be useful and which information it can provide;
- Fully understand pulse programs of various complexities for 1D and 2D NMR spectroscopy;
- Use NMR spectrometers with a comprehensive knowledge of their hardware and software;
- Identify the most suitable experiments for a given problem, set up optimized acquisition parameters, collect and process 1D and 2D spectra;
- Extract maximum information from 1D and 2D spectra and be proficient at interpretation and structural elucidation;
- Present the conclusions drawn in written and oral form.

Activities

Lectures: 44 hours
Practicals: 6 hours
Student centered learning: 76 hours
Total student effort: 126hours

Assessment

Written examination :
-Liquid-state NMR (theory): 40%
-Liquid-state NMR (structure elucidation): 25%
-Solid-state NMR (introduction): 15%
Practicals: 20%

Université de Lille

Optical spectroscopy

5 ECTS

Description

- – General introduction (1h)
- I- Rotational energy levels (2h)
  - The classical rigid rotor
  - Quantum description
- II- Rotational spectra (4h)
  - Selection rules
  - Microwave spectra of molecules
  - Isotopic effects
  - Centrifugal distorsion, rotation-vibration coupling
  - Line Intensities
- III- Non-linear molecules (4h)
  - Spheric and symetric tops
  - Asymetric tops
- IV- Determination of the geometrical structure of a molecule. (1h)
- V- Vibrational spectroscopy of diatomic molecule (6h)
  - Classical harmonic oscillator.
  - Quantum mechanics : molecular vibration as an harmonic oscillator
  - Anharmonic vibrations and the Morse oscillator.
  - High-Order anharmonicity and the Dunham expansion.
  -Bond dissociation energy
  -Rotational structure in vibrational spectra of diatomics.
- VI- Molecular symmetry and point group determination (4h)
- VII- Vibrational spectroscopy of polyatomic molecules (8h)
  - General expression of vibration
  - Linear coupling between 2 vibrators
  - Representation of vibrational normal modes, choice of coordinates
  - Projection operator method
  - Quantum treatment and quantification
  - Selection rules in Raman scattering and infrared absorption
  - Functional groups and method for spectrum analysis
- - VIII- Electronic absorption spectroscopy (8h)
  - Franck Condon principle
  - Progression and sequences, Deslandres tables
  - Rotational treatment
  - Molecular orbitals and electronic states, selection rules
  - Electronic absorption spectra
  - Coupling between vibrational and electronic states

Aims

- Calculation of rotational energy levels of linear and non-linear molecules and prediction of pure rotational and ro-vibrational spectra;
- Interpretation of spectra and determination of geometric structures;
- Group theory and vibrational spectroscopy of polyatomic molecules;
- Electronic absorption spectroscopy: Franck-Condon principle, symmetry of molecular orbitals and of electronic states, selection rules, coupling between vibrational and electronic states;
- Learning of experimental techniques (infrared and Raman spectrometers);
- Use of computer software dedicated to the calculation of spectroscopic constants and the prediction of spectra.

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 absorption and emission spectroscopy.
- Critically evaluate applicability of specific spectroscopic techniques to solve particular structural or kinetic problem.
- Review the available types of the optical spectrometers and methods of the detection of electromagnetic radiation.
- Discuss the application of software in data acquisition, assignment of molecular species and structure determination
- Interpret the results of spectral data and present the conclusions in written and oral form.

Activities

Lectures: 38 hours
Practicals: 12 hours
Student centered learning: 30 hours
Total student effort: 80 hours

Assessment

Written examination (70%)
Lab reports (30%)

X-ray diffraction
5 ECTS

Description

This course focuses on crystallography and diffraction techniques. It is divided into two parts:

Part 1: theoretical aspects of the X-ray diffraction

- X-ray generation, X-ray sources, interactions of X-rays with matter
- Diffraction principles, Bragg's law
- Crystal shapes, Bravais lattices and unit cells determination, reticular plane and Miller indices
- Symmetry in crystal, symmetry elements and operations
- Point groups and space groups, crystallographic tables
- notions on reciprocal lattice/reciprocal space, Ewald sphere
- Experimental measurements of single crystal, structure factors
- Symmetries and allowed or forbidden reflexions

Part 2: technical aspects and processing of powder diffractograms

- Powder diffractometers: X-ray sources, monochromators, detectors
- Debye-Scherrer geometry, Guinier or Seeman-Bohlin geometry. Powdered sample preparation.
- Powder diffractogram generalities, PDF data base, qualitative phase identification and potential problems, solid solution study
- Pattern Indexation, Lattice parameters and space group determination. Quantitative analysis and the Rietveld method. Grain size and micro strain measurements

Laboratory (per group of 6 persons max 3h): X-ray diffractometers presentation

Computer analysis of powder diffraction data (per group of 8 persons max 9h): Phases identification, cell parameters determination and refinement, X-ray diagrams indexing, semi-quantitative analysis, solid-solution study, grains size determination.

Additional Work:

- Report for practicals: results presentation and analysis
- Bibliographic research and synthesis: report redaction about a given topic

Aims

The aims of this unit are:

- To give a solid background on basic crystallography;
- To give a solid background in diffraction techniques;
- To highlight modern advances in XRD instrumentation and techniques.

Outcomes

After completing this unit the student should be able to cope with:

- Structural problems in ordered solid.
- Phase identification problems in:
  - crystalline powders: single phase / polyphasic materials.
  - glass ceramics.
- Solid solutions characterisation.
- Quantitative analysis.
- Characterisation of microstructrure (grain size, micro-strain).

Activities

Lectures: 22 hours
Tutorials: 6 hours
Practicals: 12 hours
Student centered learning: 77 hours
Total student effort: 132 hours

BIBLIOGRAPHY:

- *International Tables for Crystallography,* Volume A, edited by Theo Hahn, by Kluwer Academic Publishers, Dordrecht/Boston/London (1989).
- *Diffraction structure from powder diffraction data*. David, Shankland, Mc Cusker, Baerlocher. Oxford Science Publication.
- *Defect and microstructure analysis by diffraction*. Synder, Fiala, Bunge. Oxford Science Publication.
- *SolidState Chemistry and its applications*. A.R. West- John Wiley and Sons.
- *Fundamentals of Crystallography, C. Giacovazzo, H.L. Monaco, D. Viterbo, F. Scordari, G. Gilli, G. Zanotti, M. Catti, Ed. C. Giacovazzo, IURc, Oxford Science Publications.*

Assessment

Written protocol after practicals (20%)
Bibliographic report of a given topic (20%)
Written final examination (60%)

Mass Spectrometry
5 ECTS

Description

The course covers aspects of molecular mass spectrometry including the most recent developments in instrumental design, techniques and understanding of processes. The methods available for the introduction of analytical samples are presented, and the advantages and disadvantages of these methods considered. The different types of mass analyzers, their working principles and performances are discussed. Current software tools for data-dependent analysis and on-line techniques are described. Analysis applications of mass spectrometry techniques and methodologies (structure identification, quantification, imaging) in different areas of chemistry and biochemistry (small organic molecules, polymers, biomolecules as proteins, peptides or lipids) are presented and discussed.

Aims

The aims of this unit are:
• To build upon and extend the theoretical and instrumental concepts introduced during the bachelor degree programme.
• To develop the competence and confidence of the students in mass spectrometry.
• To highlight modern advances in instrumentation and techniques within mass spectrometry.
• To identify appropriate instrumentation for particular applications.

Outcomes

After completing this unit the student should be able to:

• Discuss in a comprehensive way the methods available for the introduction of samples to a mass spectrometer;
• Identify methods for ionization (sources) and ion separation (analyzers) and their advantages / disadvantages;
• Review critically the available types of mass analyzers;
• Discuss the use of software in obtaining and analyzing mass spectral data;
• Identify the most suitable instrumentation for specific applications and describe the extent and limitations of the data obtained;
• Interpret mass spectral data for various types of chemical and biochemical molecular structures, and present the conclusions drawn in written and oral form;

• Be able to use common types of mass spectrometers (experimental part), e.g. MALDI-TOF-TOF and nanoESI-Q-TOF;
• Explain to non-specialists how mass spectrometry can be expected to provide valuable information in different areas of chemistry, biochemistry and related disciplines; and know which type of complementary information it provide compared to other analytical disciplines.

Activities

Lectures: 28 hours
Practicals: 8 hours exercises + 12 hours experimental section
Student centered learning: 40 hours
Total student effort: 88 hours

Assessment

Examination on completion of teaching period:
-Written (60%)
-Oral (20%) (performed on the basis of the study of one specific actual application of mass spectrometry in private or academic domains)
-Experimental part exam (20%)

English and Professionalisation
5 ECTS

Description

The course starts with an intensive week which includes a test aimed at assessing each student's CEF level. Students who do not rate C1 or C2 are asked to work more on their English fluency.

The first part of each lesson focuses on English proficiency, through a number of oral and written documents aimed at strengthening the students' mastering of the English language (photos, videos, news clips, articles, drills).

Power point presentations are shown and discussed, each containing exercises, on each of the topics (Academic English, Presentation English, CVs, Lab English). All presentations correspond to matching exercises and drills given as homework.

Every week, free discussion is also encouraged to foster socialising inside the group, often based on news topics through news photos or BBC/Sky News/Euronews, CNN clips.

Aims

- **Academic English**: how to differentiate between spoken English and formal English, and use the appropriate terms and expressions in a formal essay/letter/thesis
- **Presentation English**: how to give good, clear and concise PP Presentation. How to prepare it, express yourself clearly, address your audience, react to questions, etc.
- **CVs and covering letters**: how to write a modern, clear, attractive CV well adapted to your goals. How to write a covering letter that will stand out and emphasise your qualities in good, accurate English
- **Lab English**: how to describe lab experiments (including materials, equipment, set up, conclusions) with audio exercises providing examples in international context
- Part of the course is also specifically aimed at students who need to improve their proficiency, with vocabulary and grammar exercises, audio and video documents, and interaction.

Outcomes

- Better mastering of the English language in professional situations linked to students' field of expertise: in the lab, presenting a project, making a PP Presentation, writing an essay, looking for a job;

- Improved self-confidence when socialising with peers from other nationalities at University and at work.

Activities

Lectures & practicals : 48 hours (intensive course 24h + weekly lessons 24h)
Student centered learning: 48 hours
Total student effort : 96 hours

Assessment

- Written comprehension and expression (2 hours) 40%;
- Oral comprehension (40 minutes) 30%;
- Oral presentation (20 minutes) 30%.