CH-314

Structural analysis

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Cursus	Sem.	Type
Chemical Engineering	BA5	Obl.
Chemistry	BA5	Obl.
HES - CGC	H	Obl.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	Written
Workload	120h
Weeks	14
Hours	**4 weekly**
Courses	3 weekly
Exercises	1 weekly
Number of positions	

Summary

The aim of this course is to treat three of the major techniques for structural characterization of molecules used in chemistry and chemical engineering: mass spectrometry, NMR, and X-ray techniques.

Content

Weeks 1-5: Mass Spectrometry (Dr. Miéville)

- introduction to molecular structures and representations
- Introduction to structure elucidaiton and verificaiton algorithms
- Introduction to mass spectrometry
- Masses of elements and molecules
- Isotopes and isotope distributions
- Fundamentals of molecular ionization processes
- Figures of merit: mass accuracy and resolution
- Mass spectrometry instrumentation: Ion sources, mass analyzers, and detectors
- Tandem MS
- Coupling MS with chromatographic methods
- Ion mobility MS

Weeks 6-10: NMR (Prof. Emsley)

- Principles of nuclear magnetism
- Quantum description of magnetic resonance leading to the vector model
- Interactions defining the spectrum: chemical shifts, scalar, dipolar and quadrupolar couplings
- Time-domain spectroscopy by pulsed excitation: interaction with radiofrequency fields, coherence, precession, signal induction and the Fourier Tranform
- Relaxation and the return to equilibrium
- Polarization transfer
- Multi-dimensional correlation spectroscopy

Weeks (11-14): X-ray (Prof. Bostedt)

- Introduction to x-rays and x-ray sources
- X-ray properties of the elements
- Diffraction and refraction
- Scattering and imaging

- X-ray spectroscopy

Keywords

Spectroscopy; Mass Spectrometry; Magnetic Resonance; NMR; X-Rays; Diffraction; Strucutre; Chemical Analysis;

Learning Outcomes

By the end of the course, the student must be able to:

- Compute the exact masses of molecules in their various ionic forms
- Use mass spectra of molecules to determine their atomic composition
- Work out / Determine the best choice of ion source and mass analyzer to solve a particular problem
- Analyze tandem mass spectra to determine the parent ion mass
- Describe the characteristic x-ray properties of the elements
- Work out / Determine a crystal structure from a diffraction pattern
- Analyze the atomic composition of a compound from its x-ray spectrum
- Explain the fundamental principles of Magnetic Resonance
- Interpret an NMR spectrum in terms of the interactions involved
- Describe the elements of a pulsed Fourier transform NMR experiment
- Design a strategy for analysis of molecular structure or dynamics by NMR

Transversal skills

- Access and evaluate appropriate sources of information.
- Set objectives and design an action plan to reach those objectives.

Teaching methods

For Mass Spectrometry and NMR: the teaching is partly reversed with external individual readings from student with complementary information during lecture time and associated exercises. Mass Spectrometry and NMR are each based on a reference book completed with power point slides and videos.

Assessment methods

Graded exercises during the semester. Written final examination.

Resources

Bibliography

- Mass spectrometry / James McCullagh and Neil Oldham
- Understanding NMR spectroscopy / James Keeler

Ressources en bibliothèque

- Retrouver les références à la Bibliothèque

Moodle Link

- https://go.epfl.ch/CH-314