

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
Lecture	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: mass spectrometry, NMR, and X-ray techniques.

Content

Weeks 1-5: Mass Spectrometry (Prof. Rizzo)

- Introduction to mass spectrometry
- Masses of elements and molecules
- Isotopes and isotope distributions
- Figures of merit: mass accuracy and resolution
- Mass spectrometry instrumentation: Ion sources, mass analyzers, and detectors
- Tandem MS
- Ion mobility MS
- Combining MS with IR spectroscopy for molecular identification

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 Transform
- 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; Structure; Chemical Analysis;

Learning Outcomes

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

Transversal skills

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

Assessment methods

Written Examination

Resources

Moodle Link

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