

Structural Analysis

CH-314

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Organizational details

Classes:

- Mondays, 14h15-17h, Rm. CH B3 30

Exercises:

- Mondays, 17h15-18h, Rm. CH B3 30

Weeks 1-5 (starts on 8th of Sept. – 4 weeks - one week off for Jeune Fédéral) :

- Dr MER P. Miéville - Mass Spectrometry

Weeks 6-11 (starts on 13th of Oct. – 5 weeks - one week off for fall break) :

- Professor L. Emsley – NMR

Weeks 12-15 (starts on 24th of Nov. – 4 weeks) :

- Professor C. Bostedt - X-ray Crystallography

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. It is largely focused on the physical chemistry of how these techniques work.

Content

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

- Different molecular representation and their information content
- Molecular structure elucidation strategies
- Introduction to mass spectrometry
- Masses of elements and molecules
- Isotopes and isotope distributions
- Mass spectrometry instrumentation: Ion sources, mass analyzers, and detectors
- Mass accuracy and resolution
- Tandem MS
- Coupling with separation techniques (chromatography) and quantification
- Ion mobility MS

Summary

Weeks 6-11: 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 12-15: 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