



# Crystallography, crystal chemistry, Large scale facilities



Niveau d'étude  
BAC +4



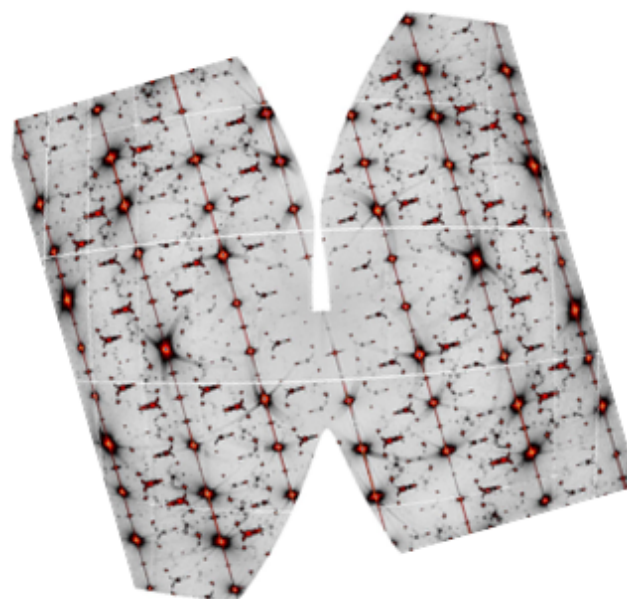
ECTS  
5 crédits



Composante  
Faculté des  
Sciences

## En bref

- › **Date de début des cours:** 1 sept. 2021
- › **Langue(s) d'enseignement:** Anglais
- › **Méthode d'enseignement:** En présence
- › **Organisation de l'enseignement:** Formation initiale
- › **Ouvert aux étudiants en échange:** Non



## Présentation

### Description



This lecture is the continuation of the crystallography lecture of the 1st semester and will give a advanced insight



into structural characterization and structure refinements. It involves classical X-ray laboratory data collection and analysis, completed by synchrotron and neutron diffraction data analysis (powder and single crystal). The goal is to get familiar with the general principles of structure analysis, taking advantage of the complementarity of X-ray and neutron diffraction. The lecture provides a detailed knowledge on how to understand and analyze phase transitions and how to deal with respective changes in the metric and associated data and structural transformations.

This lecture contains the following topics:

- \* Symmetry and space groups
- \* Introduction into structure refinement (single crystal and powder methods)
- \* Neutron and synchrotron facilities
- \* Magnetic structures with neutron diffraction
- \* Structure determination from single crystals (experiment and theory)
- \* Structure determination from powder diffraction data (experiment and theory)
- \* The applications of Fourier series for structure solution and refinements: from the Patterson Method to difference Fourier analysis
- \* Crystal twinning,
- \* Phase transitions
- \* Anomalous scattering and absolute structure determination

Volumes horaires\* :

CM : 30

TD : 15

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## Objectifs

At the end of the lecture students should be able to deal with the international Tables of Crystallography and to know how to make structure refinements from single crystal and powder diffraction data. Further on students should know how

to use neutron and synchrotron diffraction for complementary applications, and how contrast variation can be achieved by anomalous scattering or isotope substitution for synchrotron and neutron diffraction respectively.

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## Contrôle des connaissances

CC intégral

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## Syllabus

- Symmetry and space groups
- Introduction into structure refinement (single crystal and powder methods)
- Neutron and synchrotron facilities
- Magnetic structures with neutron diffraction
- Structure determination from single crystals (experiment and theory)
- Structure determination from powder diffraction data (experiment and theory)
- The applications of Fourier series for structure solution and refinements: from the Patterson Method to difference Fourier analysis
- Phase transitions, crystal twinning and related changes of the direct and reciprocal lattice
- Contrast variation and anomalous scattering together with absolute structure determination

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## Informations complémentaires

Contact(s) administratif(s) :

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## Bibliographie

- \* and C. McKie: Essentials of Crystallography, Blackwell Scientific Publications
- \* Borchardt-Ott: Crystallography: an introduction, Springer
- \* Als-Nielsen, D. McMorrow: Elements of Modern X-ray Physics
- \* Massa: Crystal Structure Determination, Springer
- \* Stout-Jensen: X-ray Structure Determination, Academic Press
- \* L. Squires : Introduction to the theory of thermal neutron scattering, Oxford, Cambridge University press
- \* Neutron and Synchrotron Radiation for Condensed Matter Studies Part I and II, Springer, Editors: Baruchel, J., Hodeau, J.-L., Lehmann, M.S., Regnard, J.-R., Schlenker, C. (Eds.)

## Infos pratiques

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### Contacts

Responsable pédagogique

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### Lieu(x)

➤ Montpellier - Triolet