

Single Crystal X-ray Diffraction.
Ross J Angel
Pavia, Autumn 2018

- Classes on Tuesdays 13:00-14:00
- First class October 2nd, then every week until December 18th, then January 8th, 15th
- Plus two classes to be scheduled
- Aula: H25 (reserved)
- 16 hours, 4 CFU

- Text book: Clegg et al. : Crystal structure analysis – principles and practice.

Syllabus

1. What is a crystal? Metric tensor and the real lattice
2. X-ray safety, diffractometer overview, experiment workflow (in lab)
3. Diffraction geometry, reciprocal lattice
4. Diffraction geometry, orientation matrix
5. Indexing (in lab)
6. Data collection theory, Ewald sphere
7. Data collection, practical aspects
8. Data reduction (in lab)
9. Intensities: theory of X-ray scattering, structure factor equation
10. Intensities: systematic absences
11. Space group determination
12. Refinement theory
13. Refinement in practice, positional parameters
14. Refinement in practice, displacement parameters
15. Refinement in practice, extinction
16. Reporting the structure