

## **Practical Aspects of Single Crystal X-ray Crystallography**

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This lecture will provide both theoretical and practical understanding of structure determination using X-ray crystallography. The course will briefly cover the basics of X-ray diffraction theory, including proper use and maintenance of the instrument, as well as offer insight into established methods for properly growing X-ray quality crystals. The main objective of the course is for students to correctly interpret the data collected from their samples, learn how to properly solve and refine X-ray data, address issues that could arise while solving, such as disorder or twinning, and ultimately prepare their data for publishing. The students will have access to X-ray data solving software emphasizing hands on learning on interpreting crystal structures.

### **Course Outline**

- 1) Basics of X-ray Diffraction (brief presentation)
- 2) Crystal Growth (online presentation)
  - i) Crystallization techniques
  - ii) Evaluation of crystals
- 3) Data Collection (taught on an individual basis)
  - i) Crystal selection
  - ii) Operation of instrument
  - iii) Data collection methods
- 4) Data Solving and Refining
  - i) X-ray structure determination
    - (a) Direct methods
    - (b) Patterson methods
  - ii) Structure refinement
  - iii) Interpretation of results
  - iv) Disorder and twinning
- 5) Publishing and Presenting Results
  - i) Crystallography tables and information files
  - ii) Crystallographic database
  - iii) Graphics

### **Course Requirements**

Masters or Ph.D. students proficient at English

### **Suggested Reading**

Werner Massa, Crystal Structure Determination, Springer