Structure Determination by X-ray Diffraction

Schedule:

Week 1: The X-ray radiation. Properties and applications. Diffraction methods in general. Fourier transformation.

Week 2: Symmetry. Structure of solid state. The crystal lattice. Miller index. Symmetry classes. Point groups. Reciprocal lattice.

Week 3: Crystals. Crystal growing, thermodynamics and kinetics. Industrial applications.

Week 4: Methods. Evolvement of X-ray diffraction methods, hardware and software. Four-circle diffractometers, sources, detectors.

Week 5: Structure determination. Main steps and their function. Unit cell, data collection, integration, point group, solution, refinement.

Week 6: Publications. Results of X-ray diffraction studies. Examples. Statistics.

Week 7: Software resources. Application of program packages APEX, WinGX, ShelX, OLEX.

Week 8: Practice. Cambridge Structural Database search, interpretation, ORTEP and MERCURY use.

Week 9: Polymorphism. Importance in pharma industry. Structural, IP and other consequences.

Week 10: The powder diffraction. Basics and applications. Neutron diffraction.

Week 11: Protein crystallography. Solution of phase problem. Ramachandran plot. Protein structure principles.

Week 12: Practice. Determination of a structure using Bruker D8 Venture diffractometer and APEX.