

Chemical Crystallography – CHE 640

Syllabus

Note: For various technical reasons, some parts of this syllabus might be rearranged. We'll cover all the same information, but perhaps in a slightly different order at the beginning.

- 1) Concepts - What are crystals and X-rays ?
- 2) Brief History
- 3) Crystal Growth
 - a) Evaporation
 - b) Slow cooling
 - c) Vapour diffusion
 - d) Solvent diffusion
 - e) Convection
 - f) Sublimation
 - g) Melt
 - h) Others
- 4) Crystal Selection
 - a) Size
 - b) Shape
 - c) General appearance
- 5) Crystal Lattices and Lattice Symmetry
 - a) Seven crystal systems
 - b) Fourteen Bravais lattices
 - c) Unit cell
 - d) Asymmetric unit
 - e) Direct and Reciprocal Lattices
- 6) X-ray Generation
 - a) Sealed tube
 - b) Rotating anode
 - c) Synchrotron
 - d) X-Ray optics
- 7) X-ray Detectors
 - a) Scintillation counters (serial diffractometers)
 - b) Area detectors
- 8) Diffraction Geometry
 - a) Bragg's law
 - b) Laue equations
 - c) Ewald sphere
 - d) Four circle geometry - "symmetric" mode serial diffractometer
 - e) Rotation geometry - modern "area detectors"
 - f) Friedel's law
- 9) Fourier Theory
- 10) Structure Factors and Electron Density

- 11) Space Group Symmetry
 - a) Hermann-Mauguin versus Schönflies notation
 - b) Inversion points
 - c) Pure rotation
 - d) Improper rotation (roto-inversion)
 - e) Mirror planes
 - f) Screw axes
 - g) Glide planes
 - h) How to read the International Tables
- 12) Data Collection
 - a) Indexing
 - b) Counting statistics
 - c) Low temperature versus room temperature
 - d) Unique data
 - e) Redundancy
- 13) Data Reduction
 - a) Lorentz and polarization corrections
 - b) Integration of intensities
 - c) Scaling and merging of intensities
- 14) Space group determination
 - a) Lattice centering
 - b) Systematic absences
 - c) Effect of lattice symmetry on the weighted reciprocal lattice
- 15) Structure Solution and the Phase Problem
 - a) Direct methods
 - b) Patterson methods
- 16) Structure Refinement
 - a) Least-squares refinement
 - b) Difference Fourier synthesis
 - c) Displacement "thermal" parameters
 - d) Hydrogen atoms
- 17) Problems
 - a) Absorption
 - b) Extinction
 - c) Thermal diffuse scattering
 - d) Renninger effects
 - e) $\lambda/2$ effects
 - f) Libration
 - g) Spherical scattering factor approximation
 - h) Disorder
 - i) Twinning
 - j) Anomalous Dispersion and Absolute Configuration
- 18) Crystallographic Literature and Databases
 - a) Thermal ellipsoid plots
 - b) Interpreting crystal structure reports
 - c) Cambridge Structure Database