

COURSE OUTLINE AND SUGGESTED READING BY SUBJECT

Structure Analysis by Single Crystal X-Ray Diffraction

Updated 2/8/09

The following topics will be covered in lectures and/or lab sessions. Suggested reading assignments correspond to chapters/sections of Stout and Jensen (SJ) or Massa (M). The reading list should be considered a guide rather than a comprehensive study program; additional reading is strongly encouraged. In particular, Stout and Jensen provides more in-depth coverage of some of the material and the appendices of Giacovazo *et al.* are very comprehensive.

| Week | Date | Lecture | Laboratory | Reading | Prob. Set. |
|------|---------|---|---|--------------|-------------------------|
| 1 | W 1/21 | Crystals, crystal lattices, unit cells, symmetry | No lab | M1, 2 SJ3 | |
| 2 | M 1/26* | Two dimensional space groups (Brown) | No lab | M6 | PS1 out |
| | W 1/28* | Diffraction of light, 2 D grating (Brown) | No lab | M3, SJ2 | |
| 3 | M 2/2 | More space group theory | Four dry lab exercises done in rotation | M4 | PS2 out, PS1 due |
| | W 2/4* | Reciprocal lattice, Miller indices, 3D space groups (DiPasquale) | Dry Lab (cont.) | SJ1 | |
| 4 | M 2/9 | Structure factor amplitudes, systematic absences | Dry lab (cont.) | M5, SJ8 | |
| | W 2/11 | Crystal quality, mounting and orientation | Dry lab (cont.) | SJ4 | PS3 out, PS2 due |
| | F | | | | |
| 5 | M 2/16 | Presidents' Day Holiday | | | PS3 due |
| | W 2/18 | First midterm | Mounting crystals and use of | SJ5 | |
| 6 | M 2/23 | X-rays and diffraction | Precession camera | | PS4 out |
| | W 2/25 | Ewald sphere, camera techniques for diffraction | Precession Lab 3 | | |
| 7 | M 3/2 | Diffraction meters, CCD detectors, data collection | Determination of crystal quality on diffractometer. | M7 | |
| | W 3/4 | Reduction of diffraction data to F ² s: absorption, etc. - | How programs work and interpretation of output. | SJ7 | PS5 out, PS4 due |

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| 8 | M | 3/9 | Fourier transforms, Electron density syntheses, difference | Computer use, dry labs on data reduction. | M8, SJ9 | |
| | W | 3/11 | Patterson function Fourier maps | Research crystal for structure determination | SJ10, 11 | PS6 out, PS5 due |
| 9 | M | 3/16 | The phase problem, thermal motion, point atoms | | | |
| | W | 3/18 | Second Midterm | Structure determination | M9, SJ16 | PS7 out, PS6 due |
| 10 | M | 3/23 | Spring recess (3/24 – 3/28) | | | |
| | W | 3/25 | Spring recess (3/24 – 3/28) | | | |
| 11 | M | 3/30 | K-H determinants, direct methods | (approximate date) Research crystal for structure determination. | | |
| | W | 4/1 | Least squares refinement | | | PS8 out, PS7 due |
| 12 | M | 4/6 | Thermal parameters, symmetry constraints | | | |
| | W | 4/8 | Distance and angle calculations, estimation of errors | Solution and refinement work using teXsan | M12, SJ18 | PS9 out, PS8 due |
| 13 | M | 4/13 | Disorder, twinning and other pathologies | Solution and refinement using SHELX. | | |
| | W | 4/15 | Third midterm | | | PS9 due |
| 14 | M | 4/20* | Synchrotron source for diffraction I (Teat) | | | |
| | W | 4/22* | Synchrotron source for diffraction II (Teat) | Visit Advanced Light Source at LBL | | |
| 15 | M | 4/27* | Protein crystallography (Kim) | | M13 | |
| | W | 4/29* | X-ray scattering of non-crystalline samples (EXAFS) (Shuh) | . | M11 | |
| 16 | M | 5/4 | Problem structures – examples of what not to do | Prepare manuscript for <i>Acta. Cryst. E</i> . | | |
| | W | 5/6 | Presentation by groups of their structures | | | |
| 17 | M | 5/11 | Presentation by groups of their structures | | | |

*guest lecturers, KR out of town