**Department of Chemistry Syllabus**

This syllabi is advisory only. For details on a particular instructor's syllabus (including books), consult the instructor's course page. For a list of what courses are being taught each quarter, refer to the Courses page. *Every instructor has prerogative to teach the course as they see fit and ultimately the instructor's syllabus supersedes all others.*

***CHE 217: X-ray Crystallography***

Approved:

Suggested Textbook: (actual textbook varies by instructor; check your instructor)

Recommended

* Sherwood, D., and Cooper, J. Crystals, X-rays and Proteins: Comprehensive Protein Crystallography. (1st ed.) (2011) Oxford University Press, Oxford UK.
* Rhodes, G. Crystallography Made Crystal Clear (3rd ed.) (2006). Academic Press, New York.

Additional Sources

* Rupp, B. Biomolecular Crystallography. (1st ed) (2010) Garland Science, New York.
* Blow, D. Outline of Crystallography for Biologists (1st ed.) (2002). Oxford University Press, Oxford.
* Drenth, J. Principles of Protein X-ray Crystallography. (3rd ed) (2007) Springer-Verlag, New York.
* Giacovazzo, C., (Ed.) Fundamentals of Crystallography. (2nd ed.) (2002) Oxford Science Publications.
* Woolfson, M. M., An Introduction to X-ray Crystallography. (1997) Cambridge University Press, Cambridge.

Suggested Schedule:

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| --- | --- | --- | --- |
| Lecture | Topic | Sherwood | Blow |
| 1 | Introduction / Linear Algebra & Matrix Review | Ch. 2 | Ch. 1 |
| 2 | Crystallization | Ch. 10 | Ch. 2 |
| 3 | Properties of crystals (density, Matthews Coef.,) mounting | Ch. 11 | Ch. 2 |
| 4 | Symmetry, Plane Groups and Space Groups | Ch. 3 | Ch. 2 |
| 5 | " " " " " | Ch. 3 | Ch. 2 |
| 6 | Symmetry and Escher Diagrams |  |  |
| 7 | International Tables and Space Group diagrams |  |  |
| 8 | X-rays and X-ray Detectors | Ch. 4, 11 | Ch. 1 |
| 9 | Scattering and Diffraction of X-rays | Ch. 6 | Ch. 4 |
| 10 | X-rays and Matter, X-ray scattering | Ch. 7 | Ch. 5 |
| 11 | X-ray Diffraction and Crystals | Ch. 8 | Ch. 5 |
| 12 | Diffraction Geometry, Bragg's Law, Reciprocal Space | Ch. 8 |  |
| 13 | Data Collection Geometry and Techniques | Ch. 8 |  |
| 14 | Space Group Determination | Ch. 5 | Ch. 5 |
| 15 | " " " " | Ch. 5 | Ch. 5 |
| 16 | Fourier Transform and Structure Factors | Ch. 9 | Ch. 6 |
| 17 | Reflection Intensities, Friedel's Law | Ch. 9 | Ch. 5 |
| 18 | Intensity Determination and Systematic Absences | Ch. 9 | Ch. 5 |
| 19 | CCP4 – Computer Lab |  |  |
| 20 | The Phase Problem | Ch. 12 | Ch. 7 |
| 21 | Fourier Transform and Electron density Calculation | Ch. 9 | Ch. 6 |
| 22 | Solving Simple 1D problems by hand |  |  |
| 23 | " " " " |  |  |
| 24 | Solving the Phase Problem, Heavy Atom & MIR | Ch. 14 | Ch. 7 |
| 25 | Solving the Phase Problem, MAD, | Ch. 14 | Ch. 8 |
| 26 | Solving the Phase Problem, Molecular Replacement | Ch. 13 | Ch. 9 |
| 27 | CCP4 – Computer Lab |  |  |
| 28 | Phase Improvement and Refinement | Ch. 15 | Ch. 12 |

Additional Notes:

Prerequisite: consent of instructor.

Learning Goals:

Introduction to x-ray structure determination; crystals, symmetry, diffraction geometry, sample preparation and handling, diffraction apparatus and data collection, methods of structure solution and refinement, presentation of results, text, tables and graphics, crystallographic literature