

Title of the course: X-ray crystallography

Kvvn9185

Credit: 2

Coordinator: Harmat, Veronika

Department: Department of Organic Chemistry

Lecturers: Simon, Kálmán and Harmat, Veronika

Pre-requisites: -

Topics covered by the course:

We discuss the bases of X-ray crystallography of small molecules and macromolecules.

1. Diffraction of X-rays
2. Theory of structure factors and Fourier synthesis
3. Symmetry of crystals and datasets
4. Direct methods
5. Structure refinement by least squares method
6. Crystallization and data collection
7. Solving the phase problem of macromolecular datasets
8. Density modification, model building
9. Refinement of macromolecular structures, maximum likelihood and molecular dynamics methods
10. Crystallographic databanks

Literature

Suggested:

C. Giacovazzo, H.L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M.Catti: „Fundamentals of Crystallography”, IUCr/Oxford University Press, 2002

JP. Glusker, M. Lewis, M. Rossi: „Crystal Structure Analysis for Chemists and Biologists”, Wiley, 1994