

Level: master				
Course title: CRYSTAL STRUCTURE DETERMINATION				
Status: elective				
ECTS: 6				
Requirements: none				
Learning objectives Obtaining knowledge on fundamentals of single crystal X-ray diffraction and advanced knowledge of practical steps in crystal structure determination.				
Learning outcomes After successfully completing the course, the student is able to: Demonstrate knowledge of single crystal X-ray diffraction methods; experimentally perform diffraction experiment; determine and refine crystal structure; validate and interpret results of structural analysis; use Cambridge Structural Database.				
Syllabus <i>Theoretical instruction:</i> geometry of X-ray diffraction. Braggs law. Reciprocal lattice and Ewald construction. Relationship between electron density and structure factor. Four circle diffractometer. Diffraction data collection and reduction. Determination of crystal system, unit cell and space group. Solutions to the phase problem. Completing and refinement of crystal structure model. Interpretation of results. Absolute structure determination. Crystallographic information file. Crystallographic databanks. Presentation of results. <i>Practical instruction:</i> Determination of crystal density. Selection and centering of crystalline specimen. Work on four-circle diffractometer. Use crystallographic programs for solution, refinement and validation of crystal structure models. Use of Cambridge Crystallographic Database. Presentation of the results.				
Weekly teaching load				Other:
Lectures: 3	Exercises: 2	Other forms of teaching:	Student research:	