

Level: bachelor				
Course title: X-Ray Structural Analysis				
Status: elective				
ECTS: 6				
Requirements: none				
Learning objectives Introduction to the theoretical foundations of the diffraction of X-rays on crystals, and basic experimental methods of the analysis of diffraction in order to solve the structure of matter.				
Learning outcomes After completing the course, students should develop: General abilities: following professional literature; use of the Internet, application in other sciences. Specific abilities: obtaining knowledge on crystal diffraction and modern techniques of collecting, measurement and analysis of the intensity of radiation scattered on crystal. Knowledge on software used in modern crystal structural analysis.				
Syllabus <i>Theoretical instruction</i> Crystals and diffraction. Generation and characteristics of x-ray radiation. Experimental detection of diffraction: the choice of the crystal and orientation. The determination of the unit cell parameters and crystal density. Space group and symmetry. Methods of registering the intensity of the diffracted ray (oscillatory, Weissenberg, precession and automatic four-circle diffractometer). Scattering on atom and group of atoms. Intensity of scattered radiation. Phase problem. Methods of structure solving. Patterson method of heavy atom. Method of isomorphous substitution. Direct method. Refinement of the parameters of the trial structure. Fourier method. Least-square method. Test of the correctness of the structure: R-Factor. <i>Practical instruction</i> Experimental exercises in the X-ray diffraction laboratory. Work with automatic diffractometer for powder and monocrystal. Practice with computer programs Fullporf and WinGX.				
Weekly teaching load				Other:
Lectures: 3	Exercises: 1	Other forms of teaching: 1	Student research:	