Course title	**Crystallography II: Diffraction methods**
Code	13.3 Chemistry 02-CRYD-11
Value	5 ECTS points
Availability	Spring semester
Prerequisites	Crystallography I: Elements
Teacher	Prof. Andrzej Katrusiak
Teaching method	15-hour lecture + 30-hour laboratory
Course description	The diffraction of X-rays constitute the practical method for determining the structure of crystals and molecules. Students will be thought the fundamental knowledge about diffraction of X-rays, neutrons and electrons, methods of retrieving the structural information from the diffraction data, and interpretation of the results. Learning outcomes: Students will be able to perform their own X-ray diffraction analysis of a crystal structure, and to competently use specialist literature.
Assessment method	Students will come to class well prepared on the material lectured before and will participate in the class discussion. Students will be asked to facilitate discussion, to raise problems, react to questions, and critique. Requirements for this course are participation in the lecture and tutorials. The final assessment is either (students choose): a paper (ca. 15 pages, 12 cpi, 1.5 spaced) on one of the topics listed or a topic of special interest that is related to class themes; or a test exam.
Syllabus:	
Week 1	Crystal symmetry – a brief repetitorium.
Week 2	Roentgen: X-rays. White and characteristic radiation. Methods of generation. Properties of x-rays and other ionisation radiation. Security measures.
Week 3	X-Ray diffraction on crystals. Fundamental Laue and Braggs experiments.
Week 4	Atomic scattering factors, form factors. Reciprocal space – unit-cell determination.
Week 5	Friedel symmetry and Lane classes.
Week 6	Systematic absences – space-group determination.
Week 7	Single-crystal diffraction methods. Basic diffractometric equipment
Week 8	Solution of crystal structures: atom-pair, direct and genetic methods.
Week 9	Crystal structure refinement – least-squares methods. H-atoms location.
Week 10	Molecular and structural dimensions, distances, angles, torsion angles, mean planes.
Week 11	Anomalous absorption and absolute configuration from X-ray data.
Week 12	Molecular and crystal graphics
Week 13	Powder diffraction – the most basic tools for materials sciences and technology.
Week 14	Neutron diffraction
Week 15	Electron diffraction and microscopy.

Literature	W. Berchardt-Ott, ”Kristallographie“, Springer Verlag, Berlin Heidelberg, 2002. C. Giacovazzo, H. L. Monaco, D. Viterbo, F. Scordari, G. Gilli, G. Zanotti, M. Catti, „Fundamentals of Crystallography”, Oxford University Press, 1992. J. P. Glusker, K. N. Trueblood, “Crystal Structure Analysis: A Primer Oxford Univ. Press. M. Van Meerssche, J. Feneau-Dupont „Introductioná la Cristallographie et á la chemie structurale“, Peeters Leuven, 1984. Richard J. D. Tilley, Crystals and Crystal Structures, John Wiley & Sons, Chichester, 2006. Also: there are very many books on chemical crystallography and diffraction methods, and students can use them – you are welcome to bring over to me the books you have available and consult then suitably for the course.