

Course title	Crystallography I: Elements
Code	13.3 Chemistry 02-CRYE-11
Value	5 ECTS points
Availability	Winter semester
Prerequisites	None
Teacher	Prof. Andrzej Katrusiak
Teaching method	15-hour lecture + 30-hour tutorial
Course description	Introduction into the subjects of symmetry, crystal structure, mineralogy, crystal habits, structure-property relations. Crystallography as the main concept of the condensed matter and its use as a basic method of chemical analysis. Learning outcome: Students will understand the symmetry of molecules and crystals and will be able to apply this knowledge generally in chemistry, physics and biology. They will learn how to use computer databases of crystal structures and programs for crystallographic calculations – they will also gain practice in reading crystallographic 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	Definitions of the crystalline state. Symmetry in nature – the concepts of symmetry.
Week 2	Crystal morphology and habits. Symmetry of confined objects: molecules and crystals.
Week 3	Point –group symmetry. International notation (Hermann-Mauguin) of crystal classes. Crystal-habit versus crystal-structure relations.
Week 4	Crystal unit cell. Translational symmetry. Nods of the crystal lattice. Bravais lattices. Crystallographic directions and their symbols.
Week 5	Stereographic projection of crystal habit and point-group symmetry. The Wulf 's stereographic net. Crystallographic planes – Miller indices.
Week 6	Matrix and quaternion representations of point-group symmetries. Schoenflies notation of point groups.
Week 7	Crystal micro-structure-symmetry, symmetry of open objects: screw axes, glide planes.
Week 8	Matrix representation of the translational symmetry elements.
Week 9	Space groups.
Week 10	Graphical representation of the space-groups symmetry. General and special positions. Symmetry-dependent and independent units.
Week 11	Chemical bonding in crystals. Coordination schemes and numbers. Atomic, ionic and van der Waals radii.

Week 12	X-Ray, electron and neutron diffraction as complementary methods in crystal structure determinations. Structure-property relations in crystals, as the basic knowledge in materials chemistry.
Week 13	Interatomic interactions. Types of crystals. Coordination schemes and numbers.
Week 14	Crystallographic computing – molecular dimensions and intermolecular interactions. Modern crystallographic computer programs as every-day tools in chemical practice.
Week 15	Crystallographic publications in scientific journals and databases.
Literature	<p>W. Berchardt-Ott, <i>Kristallographie</i>, Springer Verlag, Berlin Heidelberg, 2002.</p> <p>C. Giacovazzo, H. L. Monaco, D. Viterbo, F. Scordari, G. Gilli, G. Zanotti, M. Catti, <i>Fundamentals of Crystallography</i>, Oxford University Press, 1992.</p> <p>J. P. Glusker, K. N. Trueblood, <i>Crystal Structure Analysis: A Primer</i>, Oxford Univ. Press.</p> <p>M. Van Meerssche, J. Feneau-Dupont, <i>Introduction à la Cristallographie et à la chimie structurale</i>, Peeters Leuven, 1984.</p>