



Subject card

Subject name and code	CRYSTALLOGRAPHY, PG_00038885						
Field of study	Chemistry						
Date of commencement of studies	February 2024	Academic year of realisation of subject			2023/2024		
Education level	second-cycle studies	Subject group			Obligatory subject group in the field of study Subject group related to scientific research in the field of study		
Mode of study	Full-time studies	Mode of delivery			at the university		
Year of study	1	Language of instruction			Polish		
Semester of study	1	ECTS credits			3.0		
Learning profile	general academic profile	Assessment form			assessment		
Conducting unit	Department of Inorganic Chemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Jarosław Chojnacki					
	Teachers	prof. dr hab. inż. Jarosław Chojnacki dr hab. inż. Łukasz Ponikiewski					
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	30.0	0.0	0.0	45
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours		Self-study	SUM	
	Number of study hours	45	10.0		20.0	75	
Subject objectives	Students know basics of crystallography						
Learning outcomes	Course outcome		Subject outcome			Method of verification	
	K7_W02		Student knows basic crystallization methods. Knows and uses terms: crystallographic system and space group. He can indicate which molecular symmetry is allowed in the specific space group.			[SW1] Assessment of factual knowledge	
	K7_U01		Student can describe molecular geometry and intermolecular interactions found in the crystalline solid for the given crystallographic CIF file. Uses Cambridge Structural Database to find and compare known structures related to his structure.			[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools	
	K7_W05		He knows relations between molecular symmetry and symmetry of derived crystalline solids and their physico-chemical properties.			[SW3] Assessment of knowledge contained in written work and projects	

Subject contents	<p>Lecture: 1. Fundamentals of crystallography: crystal, unit cell, crystallographic system, indexing of nodes, directions and planes. 2. Symmetry of finite objects. Point symmetry groups. 3. Symmetry of infinite objects. Space groups. 4. Symbols of space groups. International Tables for Crystallography. 5. Practical significance of assigning space groups 6. Diffraction phenomenon. Reciprocal space. Ewald sphere. 7. Diffraction on monocrystals and powders. Analysis of diffractograms. Determination of unit cell. 8. Determination of space group based on diffraction data 9. Crystal structure determination. The phase problem. 10. Preparation of monocrystals 11. Description of typical crystal structures of elements and two-element compounds. 12. Description of structures of more complex chemical compounds 13. Typical description of crystal structures 14. Relation between physical properties and crystal symmetry 15. Determination of absolute configuration. Interpretation of measurement parameters and indices of quality of structure determination.</p> <p>Laboratory 1. Calculation of theoretical density. Stoichiometry of the elemental cell 2. Indexing planes and directions in crystals. Calculations in non-orthogonal metric systems. 3. Point groups. Construction and using group multiplication table. 4. Exercises with space group symmetry international symbols. 5. The influence of crystallization conditions on crystal growth. Principles of crystals morphology. 6. Growing crystals by sublimation or from melt. 7. Crystallization process, seeding and crystal growth rate. 8. Optical properties of crystals. Polarisation microscopy in crystallography. 9. Exercises in application of the Bragg's equation for the interpretation of diffraction patterns. 10. Assignment of Bravais lattices, Laue classes and space groups based on diffraction patterns in $hk0$ and $hk1$ layers. 11. Presentation of results of X-ray diffraction experiment 12. Description of crystal structures based on standard CIF files and reference materials taken from CSD database.</p>											
Prerequisites and co-requisites												
Assessment methods and criteria	<table border="1"> <thead> <tr> <th data-bbox="456 757 794 786">Subject passing criteria</th> <th data-bbox="799 757 1137 786">Passing threshold</th> <th data-bbox="1142 757 1481 786">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="456 792 794 822">Written exam</td> <td data-bbox="799 792 1137 822">60.0%</td> <td data-bbox="1142 792 1481 822">49.0%</td> </tr> <tr> <td data-bbox="456 828 794 857">Midterm colloquium + reports</td> <td data-bbox="799 828 1137 857">60.0%</td> <td data-bbox="1142 828 1481 857">51.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	Written exam	60.0%	49.0%	Midterm colloquium + reports	60.0%	51.0%
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Example issues/ example questions/ tasks being completed	<p>Which space groups are selected by optically pure chiral compounds? Give three examples.</p> <p>Describe symmetry operation related to a) 4-fold inversion axis b) 62 screw axis?</p>											
Work placement	Not applicable											