GDAŃSK UNIVERSITY OF TECHNOLOGY

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

<table>
<tr><td>Subject contents</td><td>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.

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 Braggs" 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.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td></td></tr>
<tr><td>Assessment methods and criteria</td><td>
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<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Written exam</td><td>60.0%</td><td>49.0%</td></tr>
<tr><td>Midterm colloquium + reports</td><td>60.0%</td><td>51.0%</td></tr>
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<tr><td>Recommended reading</td><td>
<table>
<tr><td>Basic literature</td><td>1. Z. Kosturkiewicz: Metody krystalografii. Wydawnictwo Naukowe UAM, Poznań 2000. (ISBN 83-232-1040-3)
2. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, Krystalografia. Wydawnictwo Naukowe PWN, Warszawa 2007. (ISBN 978-83-01-14704-4)
3. Z. Trzaska Durski, H Trzaska Durska, Podstawy krystalografii strukturalnej i rentgenowskiej. Wydawnictwo Naukowe PWN, Warszawa 1994. (ISBN 83-01-11388-X).</td></tr>
<tr><td>Supplementary literature</td><td>1. Muzeum Geologiczne Wydziału Nauk Geogr. Uniw. Łódzkiego, Kryształy w przyrodzie i technice, Wydawnictwo UŁ, Łódź 2005 (ISBN 83-7171-856-X).
2. P. Luger, Rentgenografia strukturalna monokryształów. PWN Warszawa 1989 (ISBN 83-01-08815-X)</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:
Krystalografia2024ChemiaMgr - Moodle ID: 37370
https://enauczanie.pg.edu.pl/moodle/course/view.php?id=37370</td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td>Which space groups are selected by optically pure chiral compounds? Give three examples.

Describe symmetry operation related to a) 4-fold inversion axis b) 62 screw axis?</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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