



Subject card

Subject name and code	Crystallochemistry, PG_00048984						
Field of study	Corrosion						
Date of commencement of studies	February 2024	Academic year of realisation of subject			2023/2024		
Education level	second-cycle studies	Subject group			Optional subject group 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	5.0		25.0	75	
Subject objectives	Students know basics of crystallography and crystal chemistry						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	K7_W01	knows meaning of basic terms in crystallography: unit cell, asymmetric unit, Miller indices of planes, symmetry in crystal. Knows basic types of inorganic structures. Knows relations between symmetry and physical properties of materials. Knows how to access quality of diffraction measurement, Can prepare description of a new crystal structure including analysis of intermolecular interactions in the solid state based on a given CIF file.			[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge		
	K7_U01	uses Mercury program for deep analyses of crystal structures. Can gather information from Crystal Structure Database. Can interpret powder diffractograms. Understands meaning of space group symbols			[SU4] Assessment of ability to use methods and tools [SU2] Assessment of ability to analyse information [SU1] Assessment of task fulfilment		

Subject contents	<p>Lecture: 1. Fundamentals of crystallography: crystal, unit cell, crystallographic system, indexing of nodes, directions and planes. Changing coordinate systems. 2. Symmetry of finite objects. Point symmetry groups. 3. Symmetry of infinite objects. Space groups. 4. Symbols of space groups. Presentation of symmetry in International Tables for Crystallography and Mercury program. 5. Practical significance of assigning space groups. 6. Diffraction phenomenon. Reciprocal space. Ewald sphere. 7. Diffraction on monocrystals and powders. Analysis of diffractograms, identification of phases and size of crystals (Scherrer equation). 8. Systematic absences. Overview of crystal structure determination. 9. Dense packing, coordination numbers. Description of typical structures of elements and chemical compounds. 10. Polymorphism and isomorphism, solid solutions. 11. Theory of crystallization, Industrial and laboratory methods for crystal growing. 12. Typical description of crystal structures. 13. Relation between physical properties and crystal symmetry. 15. Cryocrystallography and high-pressure crystallography.</p> <p>Laboratory 1. Calculation of theoretical density. Stoichiometry of the elemental cell, transformations of coordinate systems. 2. Indexing planes and directions in crystals. 3. Point groups. Assignment of symbols for given objects. 4. Exercises with space group symmetry international symbols.</p> <p>5. Exercises in application of the Laue equation for the interpretation of diffraction patterns. 6. Analysis of powder diffractograms. 7. Presentation of real X-ray diffraction experiment. 8. Searching information in CSD database and analysis of results by available computer programs. Preparation of a structural report based on the supplied CIF file.</p> <p>9. The influence of crystallization conditions on crystal growth. Principles of crystals morphology. 10. Growing crystals by sublimation or from melt. 11. Crystallization process, seeding and crystal growth rate. 12. Optical properties of crystals. Polarisation microscopy in crystallography.</p>											
Prerequisites and co-requisites												
Assessment methods and criteria	<table border="1"> <thead> <tr> <th data-bbox="453 866 794 898">Subject passing criteria</th> <th data-bbox="794 866 1142 898">Passing threshold</th> <th data-bbox="1142 866 1482 898">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="453 898 794 929">Midterm colloquium + reports</td> <td data-bbox="794 898 1142 929">60.0%</td> <td data-bbox="1142 898 1482 929">51.0%</td> </tr> <tr> <td data-bbox="453 929 794 965">Written exam</td> <td data-bbox="794 929 1142 965">60.0%</td> <td data-bbox="1142 929 1482 965">49.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	Midterm colloquium + reports	60.0%	51.0%	Written exam	60.0%	49.0%
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Written exam	60.0%	49.0%										
Recommended reading	Basic literature	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).										
	Supplementary literature	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)										
	eResources addresses	Adresy na platformie eNauczanie:										
Example issues/ example questions/ tasks being completed	<p>Based on space group symbol specify: crystal system, point symmetry of crystals and presence or absence of inversion center in structure for selected groups a) $P6_3/mmc$ and b) $I4_32_12$</p> <p>Draw schematically structure of tungsten (A2 type) and perovskite CaTiO_3.</p>											
Work placement	Not applicable											