GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Crystallography of natural compounds - from crystal isolation to structure, PG_00069254		
Field of study	Chemistry		
Date of commencement of studies	February 2025	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	2	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Inorganic Chemistry -> Faculty of Chemistry -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Jarosław Chojnacki	
	Teachers		

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

The student knows methods of isolating substances and methods of their crystallization. He/she is familiar with basic concepts of crystallography, can obtain crystals suitable for diffraction studies, and describes the structure of the compound and intermolecular interactions based on crystallographic results. He/she can use programs for structure analysis (such as Mercury, etc.).

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U02] prepares detailed documentation of the results of independently conducted experiments and analyzes the obtained results, uses professional vocabulary with understanding and prepares and communicates information	The student knows basic terms used in crystallography and can prepare a description of a new structure determined by X-ray structural analysis.	[SU5] Assessment of ability to present the results of task
[K7_K02] is able to cooperate and work in a group, taking on different roles	The student is able to collaborate and work in a laboratory group, taking on different roles within it.	[SK5] Assessment of ability to solve problems that arise in practice
[K7_U03] plans and performs the synthesis of chemical compounds with the required properties	The student performs the practical isolation of a substance from the assigned raw material and obtains crystals suitable for diffraction studies.	[SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment
[K7_W01] recognizes problems of modern chemistry, including properties and obtaining chemical compounds, necessary for making calculations, including the dependence of the compound's structure and its reactivity	The student is familiar with the problems addressed by modern chemistry, including the basics of methods that allow for the determination of the complete 3D structure of a compound.	[SW1] Assessment of factual knowledge

Subject contents

Lecture

1. Basic concepts related to crystallography: crystal, unit cell of a crystal, asymmetric part of the unit cell, crystallographic systems, indexing of nodes, directions and plane lattice.
2. Symmetry of finite polyhedra, point symmetry groups.
3. Symmetry of translational lattice, space groups, symbolism of space groups, importance of knowing the space group.
4. The phenomenon of diffraction, reciprocal lattice, Ewald sphere, diffraction on single crystals and powders, analysis of diffraction patterns, determining structures.
5. Obtaining single crystals, methods and conditions for crystallizing compounds of natural origin, physical properties of crystals and their symmetry.
6. Description of typical structures of ionic and molecular crystals in natural-origin chemical compounds, the method of presenting the description of crystal structures.
7. Determining absolute configuration and interpreting measurement parameters and quality indicators of the solution. High-pressure crystallography.
8. Applications of neutron diffraction and electron diffraction.

Laboratory

1. Determination the theoretical density of a crystal, stoichiometry in the unit cell, determining the indicators of planes and network lines.
2. Geometric calculations in oblique coordinate systems, point groups, using the group operation table, assigning point groups to given objects.
3. Investigating the impact of crystallization conditions on crystal growth, the crystallization process, saturated and supersaturated solutions, nucleation versus crystal growth, crystallization of mixtures, gel crystallization, sublimation crystallization, melt crystallization, diffusion crystallization, and hanging drop crystallization.
4. Isolation and crystallization of compounds from natural sources (ascorbic acid, citric acid, table salt, urea, niacin, cream of tartar, lysozyme isolated from chicken egg).
5. Basic description of crystal morphology, optical properties of single crystals, the use of a polarizing microscope in studying single crystals, birefringence.
6. Bragg's equation in diffraction calculations, laser light diffraction on fabrics and diffraction grating, and X-rays on crystals.
7. A demonstration of the measurement process of a monocrystal on a diffractometer with an imaging plate as a detector (IPDS).
8. Visualization and analysis of the structure using the Mercury program.
9. Description of the given structure, based on the standard CIF (crystal information file) using available computer programs and the Cambridge database (CSD).

Prerequisites and co-requisites

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
report from an indiwidually assigned task: on isolation, crystallization and structure determination	55.0%	10.0%
laboratory reports	60.0%	40.0%
test based on lecture content	55.0%	50.0%

Recommended reading

Basic literature	1. J. Chojnacki: Wstęp do krystalografii. Wydawnictwo Naukowe PWN, Warszawa 2025, (ISBN 978-83-01-23982-4) 2. Z. Kosturkiewicz: Metody krystalografii. Wydawnictwo Naukowe UAM, Poznań 2000. (ISBN 83-232-1040-3) 3. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, Krystalografia. Wydawnictwo Naukowe PWN, Warszawa 2007. (ISBN 978-83-01-14704-4) 4. Z. Trzaska Durski, H Trzaska Durska, Podstawy krystalografii strukturalnej i rentgenowskiej. Wydawnictwo Naukowe PWN, Warszawa 1994. (ISBN 83-01-11388-X).
Supplementary literature	In Polish: 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	

Example issues/ example questions/ tasks being completed	Describe the appearance of the diffraction image a) of a single crystal b) of a powdered (polycrystalline) sample. In which space groups do optically pure enantiomers crystallize? What is the physical nature of halogen bonding? Provide examples. Laboratory task: obtain crystals of citric acid and determine its structure using X-ray structural analysis.
Work placement	Not applicable

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