Crystallochemistry

Educational subject description sheet

Basic information

Study programme Chemia (General Chemistry) **Speciality** - **Organizational unit** Faculty of Chemistry **Study level** First-cycle programme **Study form** Full-time **Education profile** General academic	**Didactic cycle** 2023/24 **Subject code** 02CENS.14O.01822.23 **Lecture languages** English **Course type** Obligatory **Block** general subjects

Subject coordinator	Agnieszka Janiak
Lecturer	Agnieszka Janiak

Period	**Activities and hours**	**Number of ECTS points**
Semester 3	• Lecture: 15, Graded credit • Laboratories: 30, Graded credit	4

Goals

Code	Goal
C1	Providing students with knowledge of fundamental characteristic of the crystalline state and methods used to describe crystal structures.
C2	Developing the ability to determine the symmetry of objects (molecules, crystals) and the use of appropriate notations to describe it.
C3	Providing students with knowledge about the relationship between the crystal structures and their properties.
C4	Developing the ability to use crystallographic terms with understanding.
C5	Providing students with knowledge about the structure of elements and simple chemical compounds in the crystalline state, and the basic principles of crystal packing.
C6	Developing the ability to describe the crystal structures of elements and simple chemical compounds.

Entry requirements

No prerequisites required.

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge – Student:			
W1	knows and understands the nature of the crystalline state, fundamentals of symmetry, symmetry operations and symmetry elements.	CEN_K1_W03, CEN_K1_W08	Written colloquium, Oral colloquium
W2	knows and understands matrix representations of symmetry operations, and symmetry constraints by the space lattice.	CEN_K1_W07	Written colloquium, Oral colloquium
W3	knows and understands the description of the structure of chemical molecules and crystals in terms of symmetry and the Hermann-Mauguin and Schoenflies notations.	CEN_K1_W06, CEN_K1_W08	Written colloquium, Oral colloquium
W4	knows and understands the relationship between the crystal structure and its properties.	CEN_K1_W06, CEN_K1_W08	Written colloquium, Oral colloquium
W5	knows and understands the basic concepts of crystallochemistry.	CEN_K1_W06, CEN_K1_W07	Written colloquium, Oral colloquium
W6	knows and understands the principle of 'close-packing of spheres' in relation to the structure of metals.	CEN_K1_W06, CEN_K1_W07, CEN_K1_W08	Written colloquium, Oral colloquium
W7	knows and understands the types of chemical bonds, coordination polyhedra, efficiency of structural voids filling and stoichiometry for simple models of crystal structures.	CEN_K1_W01, CEN_K1_W06, CEN_K1_W07, CEN_K1_W08	Written colloquium, Oral colloquium
Skills – Student:			
U1	is able to use the basic concepts of symmetry.	CEN_K1_U02, CEN_K1_U13	Written colloquium, Oral colloquium
U2	is able to use the basic concepts of the space lattice.	CEN_K1_U02, CEN_K1_U13	Written colloquium, Oral colloquium

Code	Outcomes in terms of	Learning outcomes	Examination methods
U3	can describe the structure of chemical molecules and crystals in terms of symmetry and use the Hermann-Mauguin and Schoenflies notations.	CEN_K1_U02, CEN_K1_U13	Written colloquium, Oral colloquium
U4	can use the symmetry compendium (International Tables for Crystallography Vol. A).	CEN_K1_U01, CEN_K1_U02, CEN_K1_U21	Written colloquium, Oral colloquium
U5	can explain the structure of metals based on the principle of 'close-packing of spheres'.	CEN_K1_U13	Written colloquium, Oral colloquium
U6	is able to analyze the types of chemical bonds, coordination polyhedra, efficiency of structural voids filling and stoichiometry for simple models of crystal structures.	CEN_K1_U01, CEN_K1_U03, CEN_K1_U13	Written colloquium, Oral colloquium
Social competences – Student:			
K1	is ready to use the basic concepts of crystallochemistry.	CEN_K1_K02	Oral colloquium

Study content

No.	Course content	Subject learning outcomes	Activities
1.	The nature of the crystalline state, the fundamentals of symmetry, symmetry operations, and symmetry elements.	U1	Lecture, Laboratories
2.	Symmetry operations represented by matrices, symmetry constraints imposed by the space lattice.	W1, U1	Lecture, Laboratories
3.	Crystal systems, point groups and their international notation (Hermann-Mauguin). Schoenflies notation.	W3, U3	Lecture, Laboratories
4.	The space lattice: points, lines, planes; simple network symbols; Miller Indices and interplanar spacing; law of rational indices, 14 distinct Bravais lattices, the unit cell and its selection rules.	W1, U2, U3	Lecture, Laboratories
5.	Crystal structure vs. space lattice: motif, chemical composition of the unit cell, crystal density, relationship between crystal structure and its morphology.	W1, W3, U2, U3	Lecture, Laboratories
6.	Translational symmetry elements, space groups and their symbols, International Tables for Crystallography, graphic representation of space groups symmetry, general and special positions in a crystal.	W1, W3, U2, U3, U4	Lecture, Laboratories
7.	Point-group symmetry and physical properties of crystals.	W2, W4, U1	Lecture, Laboratories
8.	Fundamental of crystallochemistry, types of interactions in the crystal, crystal's classification, atomic, ionic and van der Waals radii, the main types of coordination, isomorphism, isotypes, homeotypes, polymorphism and its consequences.	W3, K1	Lecture, Laboratories
9.	The metal structure vs. the principle of close-packing of spheres'.	W4, W5, W6, U5	Lecture, Laboratories

No.	Course content	Subject learning outcomes	Activities
10.	Types of simple inorganic ionic structures vs. ionic radius ratio.	W2, W4, W5, W7, U6	Lecture, Laboratories
11.	Crystal structures of carbon allotropes.	W2, W4, W5, U6	Lecture, Laboratories
12.	Molecular crystals.	W1, W2, W5, U5, U6	Lecture, Laboratories

Additional information

Activities	Teaching and learning methods and activities
Lecture	Lecture with a multimedia presentation of selected issues
Laboratories	Discussion, Solving tasks (e.g. computational, artistic, practical), Classes method, Laboratory method, Work in groups

Activities	Credit conditions
Lecture	The written quiz (open-ended questions) is approached after obtaining a positive grade in the laboratory exercises. The grading scale with corresponding percentage distribution is as follows: • Grade 5.0 - Achieving the intended learning outcomes above 90% of the maximum possible number of points. • Grade 4.5 - Achieving the intended learning outcomes in the range of 80 - 89.9% of the maximum possible number of points. • Grade 4.0 - Achieving the intended learning outcomes in the range of 70 - 79.9% of the maximum possible number of points. • Grade 3.5 - Achieving the intended learning outcomes in the range of 60 - 69.9% of the maximum possible number of points. • Grade 3.0 - Achieving the intended learning outcomes in the range of 51-59.9% of the maximum possible number of points. • Grade 2.0 - Not achieving the intended learning outcomes; below 51% of the maximum possible number of points.
Laboratories	Obtaining a positive grade requires passing two written quizzes and a verbal presentation during the completion of exercises. The grading scale with corresponding percentage distribution is as follows: • Grade 5.0 - Achieving the intended learning outcomes above 90% of the maximum possible number of points. • Grade 4.5 - Achieving the intended learning outcomes in the range of 80 - 89.9% of the maximum possible number of points. • Grade 4.0 - Achieving the intended learning outcomes in the range of 70 - 79.9% of the maximum possible number of points. • Grade 3.5 - Achieving the intended learning outcomes in the range of 60 - 69.9% of the maximum possible number of points. • Grade 3.0 - Achieving the intended learning outcomes in the range of 51-59.9% of the maximum possible number of points. • Grade 2.0 - Not achieving the intended learning outcomes; below 51% of the maximum possible number of points.

Literature

Obligatory

1. R. Tilley, „Crystals and Crystal Structures”, John Wiley & Sons Ltd, Chichester, 2006

Optional

1. International Union of Crystallography (http://ww1.iucr.org/cww-top/edu.index.html)

Calculation of ECTS points

Activities	**Activity hours***
Lecture	15
Laboratories	30
Preparation for classes	15
Reading the indicated literature	10
Paper preparation	20
Preparation for the exam	15
Other	10
Student workload	**Hours** 115
Number of ECTS points	**ECTS** 4

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
CEN_K1_K02	The graduate is ready to understand the importance of presenting selected developments in chemistry in an accessible manner
CEN_K1_U01	The graduate can use basic chemical terminology according to IUPAC and PTChem recommendations
CEN_K1_U02	The graduate can present the knowledge acquired in an accessible manner
CEN_K1_U03	The graduate can identify and justify the properties of a substance on the basis of its structure
CEN_K1_U13	The graduate can apply basic principles of symmetry to the interpretation of crystallographic structures
CEN_K1_U21	The graduate can independently obtain information from both Polish and foreign literature, physicochemical tables and other available sources
CEN_K1_W01	The graduate knows and understands basic chemical laws and issues
CEN_K1_W03	The graduate knows and understands techniques of higher mathematics for the formal description of basic physical and chemical processes
CEN_K1_W06	The graduate knows and understands structure of molecules and crystals
CEN_K1_W07	The graduate knows and understands basic concepts of crystallochemistry
CEN_K1_W08	The graduate knows and understands the chemical properties of substances according to their structure/composition