COURSE DESCRIPTION CARD - SYLLABUS

Course name
Crystallography [S1IFar2>Krys]

Course

Field of study
Pharmaceutical Engineering

Year/Semester
3/6

Area of study (specialization)
–

Profile of study
general academic

Level of study
first-cycle

Course offered in
Polish

Form of study
full-time

Requirements
compulsory

Number of hours

Lecture
15

Laboratory classes
15

Other
0

Tutorials
15

Projects/seminars
0

Number of credit points

3,00

Coordinators

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Lecturers

Prerequisites

The student should have knowledge of the basics of inorganic, organic and psyhical chemistry, mathematics and physics. Has the necessary knowledge about raw materials and products used in chemical technology, engineering and pharmacy. The student should be able to obtain information from literature, databases and other properly selected sources.

Course objective

Providing students with the basic crystallographic laws and concepts, symmetry of molecules and crystals, and methods of describing crystal structures. Obtaining knowledge in the field of solid structure, condensed phase reactions and phase transitions occurring in it, and learning methods of morphological and diffractometric solids research. Understanding the relationship between the structural structure of a solid and its properties. Understanding the importance of solid phase in the pharmaceutical industry. Providing knowledge regarding: basic crystallographic laws and concepts, symmetry of molecules and crystals, methods of describing crystal structures and classification of crystalline bodies. Developing skills: using crystallographic terms, using the commonly accepted symbols of Hermann-Maugin and Schoenflies used to determine the symmetry of molecules and crystals

Course-related learning outcomes

Knowledge:

1. The student has general knowledge about the structure of solids and solid-state reactions in various phase systems [K_W1]
2. The student has knowledge of physics and crystallografhy to the extent enabling the describtion of crystal structure, phase transitions and polymorphs in condensed phase [K_W3]
3. The student has ordered, theoretically founded general knowledge to the extent that allows the analysis of intermolecular interactions in crystals and the description of diffusion processes and solid state reactions [K_W4]
4. The student has knowledge of the methods of characterizing solids, in particular morphology and supermolecular structure [K_W7]
5. The student has knowledge of the basic conceptual categories and terminology used in crystallography [K_W9]
6. The student has knowledge about the development of crystallography and research methods used in crystallography [K_W14]

Skills:

1. The student has the skills to obtain information from literature and databases enabling the determination of solids structure using modern research techniques [K_U1]
2.The student uses crystallographic terminology correctly [K_U3]
3. The student has knowledge related to the use of X-ray diffraction in identification tests of solids [K_U11]
4. The student has the skills to plan and carry out selected reactions in the solid phase and to describe physicochemical phenomena during their course (diffusion, phase transitions) - [K_U12]
5.The student uses computer programs supporting the implementation of tasks typical for explaining the symmetry of molecules and crystals [K_U19]

Social competences:

1. The student understands the need for further training and raising their professional competences [K_K1]
2. The student is able to work in a group and is ready to lead a team [K_K2]
3. The student is aware of the importance of the effects of engineering activities, including environmental impact [K_K3]

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Lectures: The knowledge acquired in the course is verified in the form of a written exam consisting of open and closed questions. The exam covers material from lectures, laboratories and tutorials. Passing threshold: 60%
Laboratory classes: during every class, the student's knowledge (discussion form), the performance of tasks and report compilation are assessed. The knowledge is verified in the form of a final, written test. Passing threshold: 60%.
Tutorials: Skills acquired during the tutorials are verified on the basis of the final test. Passing threshold: 50% of points.
If it won't be possible to conduct the exam and tests in the stationary form, the exam/test will be done in the form of an on-line test using the elearning platforms available at Universities.

Programme content

The program covers the following topics:
1. Crystallography as a science.
2. Description and classification of molecules and crystals.
3. Elements of symmetry of crystalline forms and self-symmetry of molecules.
4. Elements of symmetry acting within crystals.
5. Elements of symmetry in the matrix approach, symmetric equivalent points.
6. Crystal engineering.
7. Solid-state reactions.
8. Phase equilibria in solids, phase transitions.
9. Diffusion in a condensed phase.
10. Phenomenological description of the crystallization process.
11. Relationship between the structure and properties of a condensed phase.
12. X-ray diffraction from a crystal structure.

Course topics

1. Development of crystallography as a science; basic definitions, laws and concepts.
2. Description and classification of molecules and crystals with respect to symmetry.
3. Symmetry elements of crystal forms (crystal morphology) and self-symmetry of molecules - symmetry about a point, line and plane, inversion axes, combinations of symmetry elements - point groups, crystallographic systems, Hermann-Maugin and Schoenflies notation.
4. Symmetry elements operating inside the crystals - translation, screw axes and glide planes, Bravais lattices, space groups, indexing lattice planes and directions, lattice points coordinates.
5. Symmetry elements in the matrix approach, symmetrically equivalent points.
6. Intermolecular forces in the crystal lattice - crystal engineering.
7. Solid phase reactions, mechanism of reaction between solids, reactions in single and multiphase systems, reactions occurring at phase boundaries, double exchange reactions, topochemical reactions, thermal solids decomposition, phase distribution kinetics, sintering and grain growth.
8. Phase equilibria in solids, phase transitions, systems of two substances showing unlimited or limited solubility in solid state - solid solutions.
9. Condensed phase diffusion, description of the diffusion process, lattice, surface and grain boundary diffusion, reaction diffusion, diffusion controlled reactions.
10. Phenomenological description of the crystallization process, stages of the crystallization process: nucleation and crystallization, homogeneous and heterogeneous nucleation, thermal and athermal nucleation, shish-kebab structure, surface and volumetric energy of the nuclei, free energy of the nucleation process, interfacial energy, critical radius of the nuclei, energy vs. nuclei radius, nucleation rate and nucleation density, crystal growth, isothermal and nonisothermal crystallization process. Polymorphism. Crystallization processes of both single crystals and macromolecular systems.
11. The relationship between the structure and properties of the condensed phase.
12. X-ray diffraction on the crystal structure, Bragg and Laue diffraction conditions. Structural tests using a horizontal and four-wheel diffractometer. Identification and quantitative analysis by X-ray diffraction in wide angles, application of the PDF-4 database in identification analysis. Studies of morphology and topography of solid surfaces by microscopic techniques.

Teaching methods

1. Lecture: multimedia presentation.
2. Tutorials: multimedia presentation illustrated with examples given on a blackboard, teamwork.
3. Laboratories: student work with the use of teaching aids that facilitate the development of spatial imagination and understanding of symmetry and crystal structures. Activating teaching methods.

Bibliography

Basic:
1. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec Krystalografia. Podręcznik wspomagany komputero , Wydawnictwo Naukowe PWN, 2007 (and previous editions).
2. Z. Kosturkiewicz Metody krystalografii , Wydawnictwo Naukowe UAM, 2004.
3. J .Dereń, J. Haber, R .Pampuch, Chemia ciała stałego, PWN,1975.
4. Ch. A. Wert, R. M. Thomson, Fizyka ciała stałego, PWN 1974.

5. W. Przygocki, A Włochowicz, Uporządkowanie makrocząsteczek w polimerach i włóknach, WNT 2006.

Additional:
1. Z. Trzaska-Durski i H. Trzaska-Durska Podstawy krystalografii , Oficyna Wydawnicza Politechniki Warszawskiej, 2003.
2. Von Meerssche, J.Feneau-Dupont, Krystalografia i chemia strukturalna, PWN, 1984.

Breakdown of average student's workload

	Hours	ECTS
Total workload	75	3,00
Classes requiring direct contact with the teacher	50	2,00
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	25	1,00