UNIWERSYTET IM. ADAMA MICKIEWICZA W POZNANIU

X-Ray structure analysis

Educational subject description sheet

Basic information

Study programme Chemistry **Speciality** - **Organizational unit** Faculty of Chemistry **Study level** Second-cycle programme **Study form** Full-time **Education profile** General academic	**Didactic cycle** 2023/24 **Subject code** 02CHSS.21P.00978.23 **Lecture languages** English **Course type** Obligatory **Block** Basic subjects

Subject coordinator	Maciej Kubicki
Lecturer	Maciej Kubicki

Period	**Activities and hours**	**Number of ECTS points**
Semester 1	• Lecture: 15, Exam; including sub-activities: ◦ Synchronous lecture: 15 • Laboratories: 30, Graded credit	5

Goals

Code	Goal
C1	Basic knowledge allowing experimental studies on internal structure of crystals.
C2	The effects of diffraction of the radiation on the crystal lattice; the reciprocal lattice.
C3	Basics of computational methods involved in the crystal structure determination.
C4	Preparation of short reports on the experimental results.

Entry requirements

No prerequisites required.

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge – Student:			
W1	knows how to describe the crystal lattice, including Miller indices, and how to draw and read the symmetry elements of the space group.	CHS_K2_W02, CHS_K2_W04	Written exam
W2	knows the basics of diffraction of X-rays including Laue's and Bragg's equations.	CHS_K2_W02, CHS_K2_W04	Written exam
W3	knows how to calculate the structure factor and how to predict the systematical extinctions for given space group.	CHS_K2_W02, CHS_K2_W04, CHS_K2_W09	Written exam
W4	has the basic knowledge of the techniques of X-ray generation, the properties of X-rays and the safety regulations.	CHS_K2_W02, CHS_K2_W04	Written exam
W5	understands the phase problem and knows the methods of solving it.	CHS_K2_W02, CHS_K2_W04	Written exam
Skills – Student:			
U1	is able to characterize the crystalline state, to show and describe the symmetry of the external shape of the crystal.	CHS_K2_U06, CHS_K2_U11	Written colloquium, Report, correction of laboratory work
U2	is able to plan the diffraction experiment, to choose the appropriate crystal.	CHS_K2_U02, CHS_K2_U06	Written colloquium, Report, correction of laboratory work
U3	has the skills allowing to interpret the results of X-ray structure determination.	CHS_K2_U02, CHS_K2_U04	Written colloquium, Report, correction of laboratory work
U4	is able to critically analyze the published results of the structural X-ray analysis and to retrieve such data from the databases.	CHS_K2_U02, CHS_K2_U05, CHS_K2_U07	Written colloquium, Report, correction of laboratory work
U5	is able to apply safety rules in laboratory work.	CHS_K2_U15	Written colloquium, Report, correction of laboratory work

Study content

No.	Course content	Subject learning outcomes	Activities
1.	Crystalline state, symmetry, point groups. History of crystallography.	W1	Lecture, Synchronous lecture
2.	Crystal lattice, Miller indices, Bravais lattice, translational elements of symmetry, space groups.	W1, W2, U1	Lecture, Laboratories, Synchronous lecture
3.	Diffraction, interference, Laue theory, Braggs theory.	W2, U2	Lecture, Laboratories, Synchronous lecture

No.	Course content	Subject learning outcomes	Activities
4.	Atomic scattering factor, structure factor, Friedel’s law, Laue classes, systematic absences.	W3, U2, U3, U5	Lecture, Laboratories, Synchronous lecture
5.	X-rays generation, tubes, synchrotron, properties of X-rays, monochromatization, absorption.	W4, U3, U4, U5	Lecture, Laboratories, Synchronous lecture
6.	Policrystalline methods, identification of phases.	W5	Lecture, Synchronous lecture
7.	Phase problem, Patterson method, direct methods. Fourier maps.	W5, U4	Lecture, Laboratories, Synchronous lecture
8.	X-ray structure determination in practice: from crystal selection to structure refinement.	U4, U5	Lecture, Laboratories, Synchronous lecture
9.	Analysis of the results: coordinates, geometry, interactions. Graphical presentation.	U4	Laboratories
10.	Structural databases: CCDC, PDN etc.	W2, U2	Lecture, Laboratories, Synchronous lecture

Additional information

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

Activities	Credit conditions
Lecture	Final grade will be assigned based on assessment of laboratory exercises and written examination. To pass the course at least 4 (out of 5) laboratory exercises must be completed. Grading scale with applied percentage distribution: • excellent (5.0): achievement of the student's expected learning outcomes at a minimum of 90.0%. • very good (4.5): achievement by the student of the desired learning outcomes ranging from 80.0% - 89.9%. • good (4.0): achievement of student learning outcomes 70.0% - 79.9%. • average (3.5): achievement of student learning outcomes 60.0% - 69.9%. • satisfactory (3.0): attainment of the student learning outcomes within 50.0% - 59.9%. • unsatisfactory (2.0): failure of the student to achieve the expected learning outcomes below 50.0%.
Laboratories	To complete a laboratory exercise a pre-lab quiz must be passed and a satisfactory laboratory report from the experiment work must be handed in due time. Grading scale with applied percentage distribution: • excellent (5.0): achievement of the student's expected learning outcomes at a minimum of 90.0%. • very good (4.5): achievement by the student of the desired learning outcomes ranging from 80.0% - 89.9%. • good (4.0): achievement of student learning outcomes 70.0% - 79.9%. • average (3.5): achievement of student learning outcomes 60.0% - 69.9%. • satisfactory (3.0): attainment of the student learning outcomes within 50.0% - 59.9%. • unsatisfactory (2.0): failure of the student to achieve the expected learning outcomes below 50.0%.

Literature

Obligatory

1. C. Hammond, The basics of crystallography and diffraction, Oxford University Press (3rd ed.), 2009.

Optional

1. Course materials can be downloaded from the web-page of the Department of crystallography.

Calculation of ECTS points

Activities	**Activity hours***
Lecture	15
Laboratories	30
Preparation for classes	30
Report preparation	30
Preparation for the exam	45
Student workload	**Hours** 150
Number of ECTS points	**ECTS** 5

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
CHS_K2_U02	The graduate can analyze the physicochemical properties of substances based on the selection of appropriate methods and tools
CHS_K2_U04	The graduate can interpret technological diagrams and carry out technological processes on a laboratory scale
CHS_K2_U05	The graduate can use mathematical methods in calculations for complex chemical and physicochemical systems and to evaluate the obtained results critically
CHS_K2_U06	The graduate can use analytical and instrumental techniques to describe the qualitative and quantitative interpretation of chemical phenomena
CHS_K2_U07	The graduate can prepare a final report on conducted research projects and conduct a critical analysis of experiments
CHS_K2_U11	The graduate can present a complex chemical or physicochemical problem and propose a solution
CHS_K2_U15	The graduate can work in a group, performing various roles, including a leader
CHS_K2_W02	The graduate knows and understands concepts and relationships allowing for a quantitative description of complex physico-chemical phenomena
CHS_K2_W04	The graduate knows and understands physico-chemical properties of chemical compounds and materials depending on their structure / composition
CHS_K2_W09	The graduate knows and understands the ethical, legal and economic conditions applicable in the field of chemical sciences