Name: ***Modern diffraction methods in crystalline state investigations (C-PS.II2-MDMCryst)***
Name in Polish:
Name in English: ***Modern diffraction methods in crystalline state investigations***

Information on course:

Course offered by department: Faculty of Chemistry
Course for department: Faculty of Chemistry

Default type of course examination report:

Grading

Language:

English

Description:

Lecture
1. Modern devices for diffraction investigation
2. The fundamentals of qualitative diffraction analysis - analysis and applicationsof ICDD database
3. The fundamentals of quantitative diffraction analysis:
The simple comparision method
The internal standard method
RIR method
4. The Rietveld method - fundamentals relations, computer programs for Rietveld method, strategy in this method and quantitative analysis by Rietveld method.
5. Indexing of powder diffractograms - algortims and computer programs
analysis
6. The accurate determination of lattice constants
7. Determination degre of crystallinity

Laboratory

1. X-ray diffraction qualitative analysis of the one-and two-phases
samples: the basics of X-Rayan program, crystallographic databases
2. X-ray diffraction qualitative analysis of the multiphase samples
3. X-ray diffraction quantitative analysis :Simple comparison method
4. X-ray diffraction quantitative analysis : Internal standard method
5. Degree of crystallinity for polymer samples: WAXSFIT program
6. Degree of crystallinity for polyurethane samples: Influence of the
content of stiff and flexible mers on degree of crystallinity of block polymers
7. Rietveld Refinement: Refinement of powder diffractogram
8. Rietveld refinement: Qualitative analysis of two-phase samples
9. Precise determination of lattice constants:Determination of accurate
lattice constants for SMR-76 standard and for chosen zeolite samples.

Bibliography:

1. Bernard Denis Cullity, Bogdan Kołakowski, Maria Lefeld-Sosnowska, Ludwik
Górski-Podstawy dyfrakcji promieni rentgenowskich
2. Robert Alan Young-The Rietveld method
3. Jenkins R., Snyder R.: Introduction to X-Ray Powder Diffractometry

Learning outcomes:

KNOWLEDGE
W1- Have knowledge of the description and classification of the symmetry of finite objects and infinite structured objects as well as of methods of their study.
W2 - Know the theoretical fundamentals of the operation of scientific apparatus in scientific disciplines relevant to the chemistry course.

SKILLS
U1 - Be able to independently describe and classify the symmetry of crystal molecules and lattices as well as to analyze diffraction measurements.
U2 - Be able to use crystallographic databases and selected computer programs to describe the symmetry of molecules and crystals
U3 - Be able to prepare documents and reports presenting outcomes achieved in classes as well as on a specific assigned topic.

ATTITUDES

K1 - Know the limitations of his/her knowledge and understand the need of further education and also be able to inspire the learning process in others, in particular in the area of natural sciences.
K2 - Be able to work in a team and understand the need of teamwork in research in the field of modern chemistry.

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Contact hours (work with an academic teacher) 45

Total number of hours with an academic teacher 45

Number of ECTS points with an academic teacher 1.5

Non-contact hours (students' own work) 45

Total number of non-contact hours 45

Number of ECTS points for non-contact hours 1.5

Total number of ECTS points for the module 3

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Written exam – W1,W2,
Written tests – U1,U2,U3
Activity – K1,K2

Requirements

Basic knowledge in crystallography

Course credits in various terms:

<without a specific program>

Type of credits	Number	First term	Last term
European Credit Transfer System (ECTS)	3	14/15L	