Name: ***Crystallography (C-PS.II1-CRYST)***
Name in Polish:
Name in English: ***Crystallography***

Information on course:

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

Default type of course examination report:

Examination

Language:

English

Description:

Lecture

1.determination of molecular symmetry, symmetry elements, symmetry transformations, point groups, Schoenflies i Hermann-Mauguin notation;
2. stereographic projection, crystal forms, determination of molecular symmetry, coexistence of symmetry elements, crystal systems;
3. symmetry of two-and three-dimensional lattice, translational symmetry elements, Bravais lattices, notation of crystallographic space groups;
4. models of close packing in space, description of crystal lattice, indexing of crystal planes and directions, determination of coordination numbers and polyhedra, the Magnus rule;
5. two-dimensional groups and graphic visualization of space group symmetry for class mm2, basic crystallographic calculations (density, interatomic distance);
6. visualization of molecular and crystal structure using molecular graphics software (Diamond);
5. X-ray diffraction qualitative analysis, exploring powder diffraction pattern using special software (XRAYAN), identification of simple single phase samples;
6. X-ray diffraction qualitative analysis – identification of multiple phases in unknown samples (XRAYAN);
7. Rietveld method – introduction to crystal structure refinement, basics of method, exploring the software possibilities
8. performing simple calculations using Rietveld method;
10. Rietveld method – calculation of theoretical powder diffraction patterns using the structural data, studying the effects of various parameters on the powder pattern chang

Laboratory

- Determination of molecular symmetry, symmetry elements, symmetry transformations, point groups (notation);
- Stereographic projection, crystal forms, determination of molecular symmetry, coexistence of symmetry elements, crystal systems;
- Symmetry of two-and three-dimensional lattice, translational symmetry elements, Bravais lattices, notation of crystallographic space groups;
- Models of close packing in space, description of crystal lattice, indexing of crystal planes and directions, determination of coordination numbers and polyhedra;
- Basic crystallographic calculations (density, interatomic distance);
- X-ray diffraction qualitative analysis, exploring powder diffraction pattern using specialsoftware (XRAYAN), identification of simple single phase samples;

Bibliography:

1. W. Borchardt-Ott, ”Crystallography”, Springer, Berlin 1995
2. M. J. Buerger “Elementary crystallography”, John Wileh and Sons, New York, 1956
3. W. Kleber “An introduction to crystallography”, VEB Verlag Technik, Berlin, 1970.

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.

missing attribute description in English

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) 105

Total number of non-contact hours 105

Number of ECTS points for non-contact hours 3.5

Total number of ECTS points for the module 5

missing attribute description in English

W1, lecture - written test, laboratory - tests
W2, lecture- written test, laboratorium - tests

U1, lecture- written test, laboratorium – tests

K1, lecture- written test, laboratorium – tests

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)	5	15/16	