ЦЕНТЪР ЗА ОБУЧЕНИЕ – БАН

1000 София
ул. „Сердика“ № 4
http://edu.bas.bg

email: tdc-phd@cu.bas.bg
тел.: 02 987 31 67
02 979 52 60

Basic Information:

Course Title: **X-RAY STRUCTURAL ANALYSIS**

Lecturer: Rusi Rusev, Assoc.prof. Dr. (PhD)
Phone: 02 9797055, Mob. 0894 292 629
Email: r.rusev93@imc.bas.bg

Lecturer: Rosica Nikolova, Professor, Dr. (PhD)
Phone: 02 9797055, Mob. 0885 099 158
Email: r.rusev93@imc.bas.bg

Lecturer: Boris Shivachev, Professor, Dr. (PhD)
Phone: 02 9797055
Email: blshivachev@gmail.com

Total Teaching Hours: 30 lectures + 30 practical

Annotation

The course aims to give basic knowledge on X-ray structural analysis. Three main topics related to the determination of the crystal structure of new substances are discussed: symmetry of crystal structures, X-ray diffraction, crystal structure determination and refinement. Practical exercises include working on single crystal and powder diffractometers situated in the XRD laboratory where students may use their own crystal or substances to determine their crystal structures and to prepare their data for publication.

Course content

Lectures

Module 1: Crystal symmetry (12 hours) – includes the topics: Periodicity, translational symmetry, unit cell, crystal systems; Elements of symmetry; Point groups of symmetry; Space groups of symmetry, Bravais lattices; Space groups of symmetry, symbols, crystallographic tables; Main types of crystal structures.

Module 2: X-ray diffraction (10 hours) – includes the topics: X-ray radiation – basic concepts; Inverse/reciprocal space; Diffraction conditions, Laue equation, Bragg equation, Ewald sphere; Structural scattering factors; Systematic extinctions and space group of symmetry.

Module 3: Determination of crystal structure (8 hours) – includes the topics: Single crystal and powder method; Diffractometric experiment; Methods for determining crystal structure; Data preparation for publication

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Laboratory exercises

All exercises are conducted according to the lecturer's instructions and are aimed at consolidating and applying the theoretical foundations of the lectures.

1. Crystal symmetry (8 hours) – Periodicity, translational symmetry, unit cell, crystal systems; Elements of symmetry, Point groups of symmetry, Space groups of symmetry, Bravais lattices; Crystallographic tables.

2. X-ray diffraction (4 hours) – Inverse/reciprocal space; Diffraction conditions, Laue equation, Bragg equation, Ewald sphere; Scattering structural factors; Systematic extinctions and symmetry space group

3. Crystal structure determination (16 hours (4x4)) – Sample preparation and single crystal experiment; Presentation of software for determining, specifying and describing crystal structure. Crystallographic databases; Determination, specification and description of the crystal structure of a new substance; Preparation of a crystal information file (.cif) for publication of the data.

Teaching and assessment methods:

- Lectures and laboratory exercises;
- Independent work with crystallographic software and databases;
- Assessment based on participation in the practical course and a written examination.

Competencies acquired as a result of training (3–5 points):

- Understanding of the fundamental principles of crystal symmetry and X-ray diffraction;
- Skills in conducting single-crystal and powder X-ray diffraction experiments;
- Skills in crystal structure solution and refinement using specialized software;
- Ability to process, interpret, and prepare crystallographic data for scientific publications.

Literature:

1. http://escher.epfl.ch/eCrystallography/
2. http://www.iucr.org/education/pamphlets/22
3. http://ww1.iucr.org/cww-top/edu.index.html
4. https://it.iucr.org
5. http://www.ccp14.ac.uk/
6. https://www.crystallography.net/cod/

Additional information

Personal laptop, mandatory completion of the laboratory practicum. Written exam