

SELECTED ASPECTS OF MODERN X-RAY STRUCTURAL ANALYSIS

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Abstract:

The aim of the lecture is to provide the PhD students, studying at natural sciences departments, an overview of contemporary X-ray structural analysis. The presented subject is exploited in many distant areas of modern technologies, materials science, crystal engineering, organic or inorganic synthesis of new chemicals, drug design, molecular biology, *etc.* It becomes necessary to be familiar with its specific technical terms, power and limitations. The proposed lecture introduces selected aspects of crystallography, usually not covered in courses at lower levels of education at Gdansk University of Technology.

1. Recapitulation of foundations of X-ray structural analysis and its recent advances (5h)
 - a. basics of X-ray diffraction
 - b. diffraction on monocrystals
 - c. the phase problem, strong and weak points of X-ray structural analysis
 - d. brief description of the apparatus used and its modern improvements
 - e. complications: twinning, disordered structures, modulated structures and quasicrystals
2. Crystal chemistry (4h)
 - a. isomorphism and polymorphism, illustration of their significance on examples taken from the pharmaceutical industry
 - b. description of hydrogen bonding in structures including the graph sets notation
 - c. intermolecular π - π stacking interactions in crystals
 - d. selected examples of basic and advanced analysis of crystal data stored at global databases: Cambridge CSD and Brookhaven PDB
3. Some specific methods of structural analysis (5h)
 - a. powder samples
 - b. high-pressure measurements
 - c. cryocrystallography
 - d. protein crystallography: use of X-ray tubes, synchrotron or free-electron laser radiation, structure solution methods, crystallization techniques *etc.*
4. Overview of advances in modern crystallography and related areas(1h)

Assessment will be based on description of the given crystal structure, supplied in the form of CIF (Crystallographic Information File). Every student will be given an individual task.

Recommended literature:

1. Mariusz Jaskólski "Krystalografia dla biologów", Wydawnictwo Naukowe Uniwersytetu im. Adama Mickiewicza, 2010, <https://www.ibuk.pl/fiszka/26633/krystalografia-dla-biologow.html> (in Polish)
2. Interpretation of crystal structure determinations, Huub Kooijman, Internet pdf file available at <http://www.cryst.chem.uu.nl/huub/notesweb.pdf>
3. Crystal Structure Determination, William Clegg, Oxford Chemistry Primers, Oxford University Press, 1998
4. Polymorphism in Molecular Crystals, Joel Bernstein, IUCr Monographs, Clarendon press, Oxford 2002
5. X-Ray Analysis and the Structure of Organic Molecules. Jack D. Dunitz, Verlag Helvetica Chimica Acta, Basel 1995.
6. International Tables for Crystallography, Volume F: Crystallography of Biological Macromolecules, Edited by Michael G. Rossmann and Eddy Arnold, First Edition 2001
7. Recent volumes of periodics: Acta Crystallographica A, B, C or D.

Termin	Dzień tygodnia	Godzina	Miejsce
29.05.2023	poniedziałek (Monday)	11.15 - 13.00	sala nr 100 / Chemia A
30.05.2023	Wtorek (Tuesday)	9.15 - 11.00	sala nr 100 / Chemia A
31.05.2023	Środa (Wednesday)	12.15 - 14.00	sala nr 211 / GG
01.06.2023	Czwartek (Thursday)	13.15 - 15.00	sala nr 360 / GG
02.06.2023	Piątek (Friday)	10.15 - 12.00	sala nr 360 / GG
05.06.2023	poniedziałek (Monday)	11.15 - 13.00	sala nr 100 / Chemia A
06.06.2023	Wtorek (Tuesday)	9.15 - 11.00	sala nr 100 / Chemia A
07.06.2023	Środa (Wednesday)	14.15 - 16.00	sala nr 222 / Chemia A