

Subject card

| Subject name and code | CRYSTALLOGRAPHY, PG_00066060 | | | | | | | | |
|---|--|---------|---|------------|----------------|---|---------|-----|--|
| Field of study | Chemistry | | | | | | | | |
| Date of commencement of studies | February 2025 | | Academic year of realisation of subject | | | 2024/2025 | | | |
| Education level | second-cycle studies | | Subject group | | | Obligatory subject group in the field of study Subject group related to scientific | | | |
| | | | | | | research in the field of study | | | |
| Mode of study | Full-time studies | | Mode of delivery | | | at the university | | | |
| Year of study | 1 | | Language of instruction | | | Polish | | | |
| Semester of study | 1 | | ECTS credits | | | 3.0 | | | |
| Learning profile | general academic profile | | Assessment form | | | assessment | | | |
| Conducting unit | Department of Inorganic Chemistry -> Faculty of Chemistry | | | | | | | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | | prof. dr hab. inż. Jarosław Chojnacki | | | | | | |
| | Teachers | | prof. dr hab. inż. Jarosław Chojnacki | | | | | | |
| | dr hab. inż. Łukasz Ponikiewski | | | | | | | | |
| Lesson types and methods of instruction | Lesson type | Lecture | Tutorial | Laboratory | Projec | :t | Seminar | SUM | |
| | Number of study hours | 15.0 | 0.0 | 30.0 | 0.0 | | 0.0 | 45 | |
| | E-learning hours included: 0.0 | | | | | | | | |
| Learning activity and number of study hours | Learning activity Participation in classes including plan | | | | Self-study SUM | | | | |
| | Number of study 45 hours | | 5.0 | | 25.0 | | 75 | | |
| Subject objectives | Students know basics of crystallography | | | | | | | | |
| Learning outcomes | Course outcome | | Subject outcome | | | Method of verification | | | |
| | [K7_U05] analyzes the functioning of devices, equipment and technological lines used in laboratories and the chemical industry | | knows the principles of operation of equipment used for diffractive structural analysis, used in laboratories and the chemical industry | | | [SU4] Assessment of ability to use methods and tools | | | |
| | [K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation | | prepares and presents structural information in the form of a written report (mini scientific publication) from structural research based on given data, using the Mercury program (or similar software). | | | [SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools | | | |
| | [K7_U02] prepares detailed documentation of the results of independently conducted experiments and analyzes the obtained results, uses professional vocabulary with understanding and prepares and communicates information | | analyzes the results obtained in crystallographic studies, uses professional terminology with understanding and prepares the most important structural information for presentation | | | [SU3] Assessment of ability to use knowledge gained from the subject [SU2] Assessment of ability to analyse information | | | |
| | [K7_W03] recognizes and describes phenomena in the field of physics, including elements of quantum mechanics, solid state physics and nuclear physics, necessary to predict the course of physical phenomena and to solve technical problems | | recognizes and describes phenomena in the field of crystallography, solid state chemistry, necessary to predict the course of physicochemical phenomena and to solve technical problems | | | [SW1] Assessment of factual knowledge | | | |

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| Subject contents | Lecture: 1. Fundamentals of crystallography: crystal, unit cell, crystallographic system, indexing of nodes, directions and planes. 2. Symmetry of finite objects. Point symmetry groups. 3. Symmetry of infinite objects. Space groups. 4. Symbols of space groups. International Tables for Crystallography. 5. Practical significance of assigning space groups 6. Diffraction phenomenon. Reciprocal space. Ewald sphere. 7. Diffraction on monocrystals and powders. Analysis of diffractograms. Determination of unit cell. 8. Determination of space group based on diffraction data 9. Crystal structure determination. The phase problem. 10. Preparation of monocrystals 11. Description of typical crystal structures of elements and two-element compounds. 12. Description of structures of more complex chemical compounds 13. Typical description of crystal structures 14. Relation between physical properties and crystal symmetry 15. Determination of absolute configuration. Interpretation of measurement parameters and indices of quality of structure determination. | | | | | | |
|--|---|--|-------------------------------|--|--|--|--|
| | Laboratory 1. Calculation of theoretical density. Stoichiometry of the elemental cell 2. Indexing planes and directions in crystals. Calculations in non-orthogonal metric systems. 3. Point groups. Construction and using group multiplication table. 4. Exercises with space group symmetry international symbols. 5. The influence of crystallization conditions on crystal growth. Principles of crystals morphology. 6. Growing crystals by sublimation or from melt. 7. Crystallization process, seeding and crystal growth rate. 8. Optical properties of crystals. Polarisation microscopy in crystallography. 9. Exercises in application of the Braggs" equation for the interpretation of diffraction patterns. 10. Assignment of Bravais lattices, Laue classes and space groups based on diffraction patterns in hk0 and hk1 layers. 11. Presentation of results of X-ray diffraction experiment 12. Description of crystal structures based on standard CIF files and reference materials taken from CSD database. | | | | | | |
| Prerequisites and co-requisites | | | | | | | |
| Assessment methods and criteria | Subject passing criteria | Passing threshold | Percentage of the final grade | | | | |
| | Midterm colloquium + reports | 60.0% | 51.0% | | | | |
| | Written exam | 60.0% | 49.0% | | | | |
| Recommended reading | Basic literature 1. Z. Kosturkiewicz: Metody krystalografii. Wydawnictwo Naukowe UAM, Poznań 2000. (ISBN 83-232-1040-3) 2. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, Krystalografia. Wydawnictwo Naukowe PWN, Warszawa 2007. (ISBN 978-83-01-14704-4) 3. Z. Trzaska Durski, H Trzaska Durska, Podstawy krystalografii strukturalnej i rentgenowskiej. Wydawnictwo Naukowe PWN, Warszawa 1994. (ISBN 83-01-11388-X). | | | | | | |
| | Supplementary literature | Muzeum Geologiczne Wydziału Nauk Geogr. Uniw. Łódzkiego, Kryształy w przyrodzie i technice, Wydawnictwo UŁ, Łódź 2005 (ISBN 83-7171-856-X). P. Luger, Rentgenografia strukturalna monokryształów. PWN Warszawa 1989 (ISBN 83-01-08815-X) | | | | | |
| | eResources addresses | Adresy na platformie eNauczanie: Krystalografia2025ChemiaMgr - Moodle ID: 44127 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=44127 | | | | | |
| Example issues/ example questions/ tasks being completed | Which space groups are selected by optically pure chiral compounds? Give three actual examples. Describe symmetry operation related to a) 4-fold inversion axis b) 62 screw axis? | | | | | | |
| | 2 Section Symmetry Specialist (Stay) Flora investigation axio by 82 Section axio. | | | | | | |
| Work placement | Not applicable | Not applicable | | | | | |

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