GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

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| Subject name and code | Methods for the structural study of substances - team project, PG_00060875 | | | | | | |
| Field of study | Chemical Technology | | | | | | |
| Date of commencement of studies | October 2024 | | Academic year of realisation of subject | 2026/2027 | | | |
| Education level | first-cycle studies | | Subject group | Obligatory subject group in the field of study<br>Optional subject group | | | |
| Mode of study | Full-time studies | | Mode of delivery | at the university | | | |
| Year of study | 3 | | Language of instruction | Polish | | | |
| Semester of study | 6 | | ECTS credits | 2.0 | | | |
| Learning profile | general academic profile | | Assessment form | assessment | | | |
| Conducting unit | Department of Organic Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology | | | | | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | | prof. dr hab. inż. Maria Milewska | | | | |
| | Teachers | | | | | | |
| Lesson types | Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
| | Number of study hours | 15.0 | 0.0 | 0.0 | 15.0 | 0.0 | 30 |
| | E-learning hours included: 0.0 | | | | | | |
| Learning activity and number of study hours | Learning activity | Participation in didactic classes included in study plan | | Participation in consultation hours | | Self-study | SUM |
| | Number of study hours | 30 | | 3.0 | | 17.0 | 50 |
| Subject objectives | A main goal is to teach students basic spectroscopic methods including: NMR, IR, and MS, and their application in the analysis of the structure of organic compounds | | | | | | |

| Learning outcomes | Course outcome | Subject outcome | Method of verification |
|---|---|---|---|
| | [K6_W02] has knowledge of inorganic, organic, physical and analytical chemistry useful for obtaining selected groups of compounds, determining their physical and chemical properties allowing for their quantitative and qualitative analysis, making measurements and determining the parameters of chemical reactions, phenomena and processes occurring in chemical technology | Student is able to apply knowledge of the basics of physical, organic and inorganic chemistry and mathematics to analyze spectroscopic spectra. | [SW1] Assessment of factual knowledge |
| | [K6_K05] is aware of the social role of a technical university graduate, and in particular understands the need to formulate and communicate to the public, in particular through the mass media, information and opinions on the achievements of technology and other aspects of engineering activity | The student is able to communicate with specialists from other fields in a clear manner and provide information on issues related to simple spectroscopic studies. | [SK4] Assessment of communication skills, including language correctness |
| | [K6_U01] is able to acquire information from literature, databases and other appropriately selected sources, also in English; is able to integrate information obtained, interpret it and make conclusions, formulate and justify opinions | The student is able to use databases and software for processing spectroscopic data. | [SU4] Assessment of ability to use methods and tools |
| | [K6_U03] is able to apply knowledge of inorganic, organic, physical and analytical chemistry and identify appropriate sources of information to design and synthesize simple chemical compounds, carry out basic physicochemical and analytical measurements | Based on NMR and IR spectra, student can identify and point out functional groups present in organic compounds; student can introduce spectroscopic and slit-scan measurements and obtain computer-generated results. | [SU1] Assessment of task fulfilment |

**Subject contents**

Course content – lecture
1. Principles of spectroscopy electromagnetic radiation, energy levels in molecules, absorption of radiation, line
shape, selection rules, application of the Fourier transformation in spectroscopy.
2. NMR magnetic properties of atomic nuclei, the chemical shift, the spin-spin coupling, diamagnetic anisotropy
of molecules, interpretation of the proton NMR spectra, spin systems, the Karplus equation, dynamic effects, the Fourier transformation (FT-NMR), basics of $^{13}C$ NMR.
3. Infrared spectroscopy (IR): harmonic and anharmonic oscillator, vibrations of multiatom molecules, the normal vibrations, transition probability, group frequencies, measurements of the IR spectra, interpretation of the IR spectra, hydrogen bonds in the IR spectroscopy.
4. Mass spectroscopy (MS): physical basis of the MS spectroscopy, methods of sample ionization including electro- ant thermospray, ion types in MS, determination of molecular mass and molecular formula, fragmentation of molecules.

Course content – project
**Project Tasks**

**Obligatory Tasks**

1. Determining the chemical purity of the student preparation obtained during the organic synthesis labs:

a) Measurement of $^{1}H$ NMR and IR spectra of an unknown sample

b) Improvement of skills in the analysis and interpretation of $^{1}H$ and $^{13}C$ NMR, IR, and MS spectra

c) Computer-assisted processing of the FID of the $^{1}H$ NMR spectrum

d) Analysis and interpretation of the obtained spectra

e) Discussion of the purity and actual composition of the preparation from the student laboratory

**Elective Tasks**

1. Design and conduct (with the assistance of an NMR operator) a spectroscopic experiment allowing for the observation of the ketone-enol equilibrium; analysis and interpretation of the obtained results, discussion of the effect of the solvent on the ketone-enol equilibrium, and determination of the ketone-enol concentration ratio.

2. Design and conduct (with the assistance of an NMR operator) a spectroscopic experiment predicting the exchange of protons for deuterons; analysis and interpretation of the obtained results, discussion of the effects of proton-deuteron exchange.

3. Design and conduct (with the assistance of an IR operator) a series of spectroscopic measurements on samples of common materials to detect compounds contained therein based on IR absorption by determining characteristic functional groups.

**Prerequisites and co-requisites**

1. Knowledge of theoretical basis of spectroscopy
2. Knowledge of structures of organic compounds
3. Knowledge of nomenclature of organic compounds

**Assessment methods and criteria**

| Subject passing criteria | Passing threshold | Percentage of the final grade |
|---|---|---|
| Midterm test NMR, IR, MS | 60.0% | 25.0% |
| Reports on research conducted | 100.0% | 50.0% |
| teoretical test | 60.0% | 25.0% |

**Recommended reading**

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| Basic literature | 1. R. M. Silverstein, F. X. Webster, D. J. Kiemle "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 2007.<br>2. "Spektroskopowe metody badania struktury związków organicznych", praca zbiorowa red. A. Rajca, WNT, Warszawa, 1996 lub 2000.<br>3. R. M. Silverstein, G. C. Bassler "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 1970.<br>4. J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks "Organic Structural Spectroscopy' Prentice-Hall, Inc., 1998 |

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|---|---|---|
| | Supplementary literature | 1. R. A.W. Johnstone, M. E. Rose "Spektrometria mas podręcznik dla chemików i biochemików", PWN, Warszawa, 2001.<br>2. A. Zschunke "Spektroskopia magnetycznego rezonansu jądrowego w chemii organicznej", PWN Warszawa, 1976.<br>3. Z. Kęcki "Podstawy spektroskopii molekularnej", PWN, Warszawa, 1972.<br>4. H. Günther, "Spektroskopia magnetycznego rezonansu jądrowego", PWN, Warszawa, 1983. |
| | eResources addresses | |
| Example issues/ example questions/ tasks being completed | 1. What characteristic of vibrational frequencies makes IR spectroscopyuseful in determining structures of organic compounds?<br>2. How many kinds of nonequivalent protons are there in (a) p-diethylbenzene (b) 1,1,4-trichlorobutane?<br>3. Which electron in most like to be lost in the ionization of the following compounds? (a) $CH_4$ (b) $H_2C=CH_2$ (c) $H_2C=O$ | |
| Practical activites within the subject | Not applicable | |

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