GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

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| Subject name and code | Spectroscopic methods for identification of organic compounds, PG_00053340 | | |
| Field of study | Biomedical Engineering, Biomedical Engineering, Biomedical Engineering | | |
| Date of commencement of studies | February 2023 | Academic year of realisation of subject | 2022/2023 |
| Education level | second-cycle studies | Subject group | Optional subject group<br>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 Chemistry and Technology of Functional Materials -> Faculty of Chemistry | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | prof. dr hab. inż. Elżbieta Luboch | |
| | Teachers | prof. dr hab. inż. Elżbieta Luboch<br>dr inż. Natalia Łukasik<br>dr hab. inż. Ewa Wagner-Wysiecka | |

Lesson types and methods of instruction

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
|---|---|---|---|---|---|---|
| Number of study hours | 15.0 | 0.0 | 15.0 | 0.0 | 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 | 2.0 | 43.0 | 75 |

Subject objectives

Acquiring the ability to use NMR and IR spectroscopy and mass spectrometry to determine the structure of organic compounds

Learning outcomes

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [K7_K02] is ready to provide critical evaluation of received content and to acknowledge the importance of knowledge in solving cognitive and practical problems | Understands the importance of knowledge in solving practical problems | [SK5] Assessment of ability to solve problems that arise in practice |
| [K7_U05] can plan and conduct experiments related to the field of study, including computer simulations and measurements; interpret obtained results and draw conclusions | Can plan experiments and interpret the obtained results | [SU3] Assessment of ability to use knowledge gained from the subject |
| [K7_W06] Knows and understands, to an increased extent, the basic processes taking place in the life cycle of devices, facilities and technical systems. | He understands the principle of operation of the apparatus used to characterize organic substances | [SW1] Assessment of factual knowledge |
| [K7_W53] Knows and understands, to an increased extent, selected aspects of biomedical diagnostics. | Has knowledge of the characterization and identification of organic substances | [SW1] Assessment of factual knowledge |

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| Subject contents | Isolation from complex post-reaction mixtures or natural raw materials and purification of preparations to obtain the desired organic compound in pure form. Introduction to spectroscopic methods. Nuclear magnetic resonance spectroscopy: theoretical basis. Proton Magnetic Resonance ($^1$H NMR): theoretical basis, ranges of chemical shifts for individual classes of organic compounds. Spin coupling. Calculation of chemical shifts for aromatic protons. Problem solving. $^{13}$C NMR spectroscopy, theoretical basis, chemical shifts and the structure of an organic compound. DEPT method. Solving sentences using, among others calculating carbon shifts in the benzene ring. 2D NMR correlation spectroscopy. NMR spectroscopy of other spin ½ nuclei. Application of the NMR method in medicine. Infrared (IR) spectroscopy theoretical introduction. Characteristic absorption bands for individual classes of organic compounds. Techniques for making IR spectra. IR spectroscopy problem solving. Mass spectrometry (MS) theoretical basis. Apparatus. Introduction to ionization methods. Electron ionization (EI): molecular ion and isotope ions, characteristic fragmentation of individual classes of organic compounds. Other ionization methods: CI method and ESI method. Problem solving. |
| Prerequisites and co-requisites | Knowledge of organic chemistry and knowledge of basic laboratory techniques |

Assessment methods and criteria

| Subject passing criteria | Passing threshold | Percentage of the final grade |
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| Laboratory: completion of three reports and one test | 50.0% | 50.0% |
| Lecture: written final test | 50.0% | 50.0% |

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><br>2. W. Zieliński, A. Rajca (red.), Metody spektroskopowe i ich zastosowanie do identyfikacji związków organicznych, WNT, Warszawa 2000.<br><br>3. J. McMurry, Chemia organiczna, PWN, Warszawa, 2003.<br><br>4. E. Białecka-Floriańczyk, J. Włostowska, Ćwiczenia laboratoryjne z chemii organicznej, Wyd. SGGW, Warszawa 2007.<br><br>5. J. Clayden, N. Greeves, S. Warren, P. Wothers, Chemia organiczna. WNT, Warszawa 2009.<br><br>6. P. Suder, J. Silberring (red.), Spektrometria mas, Wyd. UJ, Kraków 2006. |
| Supplementary literature | 1. Free spectral databases available on the Internet, eg Spectral Database for Organic Compounds SDBS |
| eResources addresses | Adresy na platformie eNauczanie: |

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| Example issues/ example questions/ tasks being completed | Application of selected chromatographic methods for the isolation and identification of organic compounds. Thin layer chromatography: general characteristics, application and principles of proper preparation of TLC plates for developing a chromatogram. Thin layer chromatography: detection methods. Preparative thin layer chromatography. Flash chromatography: what it is characterized by and what are its advantages. NMR spectroscopy: the basis of the NMR phenomenon. Which nuclear spin is the most advantageous from the point of view of NMR spectroscopy and which nuclei are of the greatest practical importance in NMR spectroscopy? NMR spectroscopy: steps in making an NMR spectrum. Explain the term "chemical shift" used in NMR spectroscopy. Commonly used chemical shift scale in NMR spectra. $^{1}$H NMR: why are aromatic proton signal shifts usually greater than that of alkenes? $^{1}$H NMR: what do proton shifts mainly depend on in aliphatic systems? $^{1}$H NMR: what do proton shifts mainly depend on in aromatic systems? $^{1}$H NMR: briefly explain the spin coupling phenomenon. Draw a fragment of the spectrum for a given proton system, eg CH-$CH_2$. If a given proton has two chemically unequal protons as neighbors, what will be the multiplicity of the proton's signal in the $^{1}$H NMR spectrum? (Refer to the appropriate figure for the answer.) Interpret the $^{1}$H NMR spectrum of 1-nitropropane (attached). Please draw a fragment of the $^{1}$H NMR spectrum containing signals from the isopropyl group that is adjacent to the oxygen atom. Please calculate the shifts of aromatic proton signals in the $^{1}$H NMR spectrum of eg salicylic acid. Most of the $^{1}$H NMR spectra are recorded for solutions in $CDCl_3$, at what shifts are to be expected in these spectra signals from non-deuterated solvent and water in this solvent? $^{13}$C NMR spectroscopy: why only single peaks in a typical $^{13}$C NMR spectrum? Characteristic areas in the $^{13}$C NMR spectrum. Interpret the $^{13}$C NMR spectrum of a simple aliphatic organic compound with the given structural formula. Interpret the $^{13}$C NMR spectrum of an organic compound containing a benzene ring with the given structural formula, calculate theoretical values of aromatic proton shifts and compare with the real ones. Solvent signals in $^{13}$C NMR spectra, their chemical shift and multiplicity (discuss on the example of selected, three popular solvents, eg $CDCl_3$, $CD_3SOCD_3$ and $CD_3OD$). Discuss the DEPT $^{13}$C NMR method in general. Interpret the $^{13}$C NMR spectra of a compound with a known structure using the basic spectrum, DEPT 135 and DEPT 90. Discuss the fundamental differences between carbon and proton magnetic resonance. 2D NMR methods: discuss the $^{1}$H-$^{1}$H COSY method. 2D NMR methods: discuss the HMQC method. Generally discuss the issue: the use of high-resolution NMR in medicine. IR spectroscopy: in general, what information can be obtained from the IR spectra? In general, what determines the frequency of stretching vibrations? Main ranges in IR spectra. Methodology of sample preparation for IR spectra. Infrared absorption of hydrocarbons. Characteristic bands in the IR spectra of alcohols (or: amines, carboxylic acids, esters, amides, nitro compounds or other discussed). Briefly discuss special methods of recording IR spectra of a solid. Mass spectrometry (MS): theoretical foundations of mass spectrometry. Discuss the method of electron ionization (EI). The way of presenting the mass spectrum. Isotope profiles in mass spectra. Determination of the atomic composition of a chemical compound by high-resolution mass spectrometry. General rules for the fragmentation of organic compounds. Fragmentation of the alkanes. Ketone fragmentation. Fragmentation of aromatic hydrocarbons. Interpret the MS EI spectrum knowing the compound's structural formula. Examples of "mild" ionization methods: discuss the CI method. ESI ionization method (general). ESI ionization method: recording of mass spectra in positive and negative ion mode. Identify a chemical compound knowing its summary formula and having a complete set of $^{1}$H NMR, $^{13}$C NMR, IR and MS spectra. |
| Work placement | Not applicable |