GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Spectroscopic methods for identification of organic compounds, PG_00068815		
Field of study	Biomedical Engineering, Biomedical Engineering, Biomedical Engineering		
Date of commencement of studies	February 2026	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	Optional subject group Specialty subject group 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	4.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Chemistry and Technology of Functional Materials -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Anna Schmidt	
	Teachers	dr hab. inż. Anna Schmidt	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	15.0	15.0	0.0	0.0	45

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	45	7.0	48.0	100

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_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
[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_U12] is able, to an increased extent, to analyze the operation of components and systems related to the field of study, as well as to measure their parameters and study their technical characteristics, and to plan and carry out experiments related to the field of study, including computer simulations, interpret the obtained results and draw conclusions	The student knows and understands the principles of operation of the apparatus used in structural studies of organic compounds. Student can plan experiments and interpret their results - determine the structure of organic compound using spectroscopic data.	[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools
[K7_W10] knows and understands, to an increased extent, the basic processes occurring in the life cycle of equipment, objects and technical systems, as well as methods of supporting processes and functions, specific to the field of study	The student knows and understands the principles of spectroscopic databases and is able to use them	[SW3] Assessment of knowledge contained in written work and projects

Subject contents	Course content – lecture General introduction to the most important spectroscopic methods. Sample preparation for analysis. Mass spectrometry (MS): theoretical foundations. Instrumentation. Introduction to ionization methods. Electron ionization (EI): the molecular ion and isotope ions, characteristic fragmentation of specific classes of organic compounds. Other ionization methods: CI method and ESI method. Problem solving. Infrared spectroscopy (IR): theoretical introduction. Characteristic absorption bands for specific classes of organic compounds. Techniques for recording IR spectra. IR spectroscopy: problem solving. Nuclear magnetic resonance spectroscopy theoretical foundations. Proton Nuclear Magnetic Resonance (^{1}H NMR): theoretical foundations: chemical shift ranges for specific classes of organic compounds. Spin-spin coupling phenomena. Calculating chemical shifts for protons: aliphatic and aromatic, located in different chemical environments. Problem solving. Carbon-13 NMR spectroscopy (^{13}C NMR): theoretical foundations, chemical shifts, and the structure of the organic compound. DEPT method. Problem solving, including, among others, the calculation of carbon shifts in a benzene ring. 2D NMR correlation spectroscopy. NMR spectroscopy of other spin-½ nuclei. Application of NMR in medicine.
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
Laboratory: completion of tests and reports	51.0%	50.0%
Lecture: written final test	51.0%	50.0%

Recommended reading

Basic literature	1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spektroskopowe metody identyfikacji związków organicznych, PWN, Warszawa 2007. 2. W. Zieliński, A. Rajca (red.), Metody spektroskopowe i ich zastosowanie do identyfikacji związków organicznych, WNT, Warszawa 2000. 3. J. McMurry, Chemia organiczna, PWN, Warszawa, 2003. 4. E. Białecka-Floriańczyk, J. Włostowska, Ćwiczenia laboratoryjne z chemii organicznej, Wyd. SGGW, Warszawa 2007. 5. J. Clayden, N. Greeves, S. Warren, P. Wothers, Chemia organiczna. WNT, Warszawa 2009. 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	

Example issues/ example questions/ tasks being completed	Mass spectrometry (MS): theoretical foundations of mass spectrometry. Discuss the electron ionization (EI) method. Representation of a mass spectrum. Isotopic profiles in mass spectra. Determination of the elemental composition of a chemical compound using high-resolution mass spectrometry. General rules of fragmentation of organic compounds. Fragmentation of alkanes. Fragmentation of ketones. Fragmentation of aromatic hydrocarbons. Interpret an EI MS spectrum given the structural formula of a compound. Examples of soft ionization methods: discuss the CI method. ESI ionization method (in general). ESI ionization method: recording mass spectra in positive-ion and negative-ion modes. IR spectroscopy: In general, what information can be obtained from IR spectra? In general, what does the stretching vibration frequency depend on? Main regions in the IR spectra. Methodology of sample preparation for IR spectra. Infrared absorption of hydrocarbons. Characteristic bands in IR spectra of alcohols (or: amines, carboxylic acids, esters, amides, nitro compounds, or others discussed). Briefly discuss special methods for recording IR spectra of solids. NMR spectroscopy: the basis of the NMR phenomenon. Which nuclear spin is most favorable from the point of view of NMR spectroscopy, and which nuclei are of the greatest practical importance in NMR spectroscopy? Chemical shifts of deuterated solvents resulting from the presence of non-exchangeable protons and water. NMR spectroscopy: sample preparation and stages of recording an NMR spectrum. Explain the concept of chemical shift used in NMR spectroscopy. The commonly used chemical shift scale in NMR spectra. ^{1}H NMR: Why are the chemical shifts of aromatic protons usually greater than those of alkenes? ^{1}H NMR: What mainly determines the chemical shifts of protons in aliphatic systems? ^{1}H NMR: What mainly determines the chemical shifts of protons in aromatic systems? ^{1}H NMR: Briefly explain the phenomenon of spin-spin coupling. Draw a fragment of a spectrum for a given proton system, e.g., CHCH. If a given proton has two chemically non-equivalent neighboring protons, what will be the multiplicity of that proton's signal in the ^{1}H NMR spectrum? (Support the answer with an appropriate drawing.) Interpret the attached ^{1}H NMR spectrum of 1-nitropropane. Draw a fragment of the ^{1}H NMR spectrum containing the signals of an isopropyl group that is adjacent to an oxygen atom. Calculate the chemical shifts of aromatic protons in the ^{1}H NMR spectrum, e.g., of salicylic acid. Most ^{1}H NMR spectra are recorded for solutions in CDCl; at what chemical shifts should one expect residual solvent and water signals in such spectra?
Practical activites within the subject	Not applicable

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