GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Spectroscopic Methods for the Identification of Organic Compounds, PG_00068087		
Field of study	Biomedical Engineering		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2027/2028
Education level	first-cycle studies	Subject group	Optional 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	3	Language of instruction	Polish
Semester of study	5	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	exam
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	prof. dr hab. inż. Ewa Wagner-Wysiecka	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	30.0	0.0	0.0	60
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	60	3.0	37.0	100

Subject objectives

The aim of the course is to introduce students to the basic spectroscopic methods (IR, Raman, NMR, MS, CD) used in the analysis of organic compounds, with particular emphasis on applications in biomedical engineering. The course aims to develop skills in using spectroscopy for chemical, pharmaceutical, and medical analyses, including quality control of biologically active substances and pharmaceutical products.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U02] can perform tasks related to the field of study in an innovative way as well as solve complex and nontypical problems, applying knowledge of physics, in changing and not fully predictable conditions	The student is able to independently and innovatively solve the basic tasks related to determining the structure of organic compounds using appropriate spectroscopic methods. The student is capable of solving analytical problems of varying difficulty.	[SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment
[K6_U09] can carry out a critical analysis of the functioning of existing technical solutions and assess these solutions, as well as apply experience related to the maintenance of technical systems, devices and facilities typical for the field of studies, gained in the professional engineering environment	The student is able to critically evaluate spectroscopic methods as a source of information about the structure of organic compounds. The student can operate basic equipment and apparatus used in spectroscopic analysis.	[SU2] Assessment of ability to analyse information
[K6_W52] Knows and understands, to an advanced extent, selected aspects of chemistry and biochemistry, constituting general knowledge related to the field of study	The student has knowledge of spectroscopic methods used in the analysis of organic compounds and their applications in biomedical engineering. The student is able to apply these methods to analyze biologically active substances and in the process of quality control of pharmaceutical products.	[SW1] Assessment of factual knowledge

Subject contents	Course content – lecture **Lecture** 1. Introduction to spectroscopic methods (IR, Raman, NMR, MS, CD) Overview of physicochemical principles and the application scope of key spectroscopic techniques used in the analysis of organic compounds. 2. Infrared spectroscopy (IR) theoretical background and spectral interpretation Types of molecular vibrations, assignment of absorption bands to functional groups, and basic principles of IR spectral analysis. 3. Raman spectroscopy and comparison with IR Physical principles of Raman spectroscopy and its application in structural identification as a technique complementary to IR. 4. Optical properties of chiral compounds fundamentals of chirality and optical activity The phenomenon of chirality, optical rotation, and the significance of absolute configuration in chemical and pharmaceutical analysis. 5. Circular dichroism (CD) application in structural studies Principles of CD spectroscopy, interpretation of CD spectra, and applications in conformational analysis, proteins, and chiral compounds. 6. Mass spectrometry (MS) ionization techniques and types of analyzers Overview of ionization techniques (EI, CI, ESI, MALDI) and mass analyzers (TOF, quadrupole, Orbitrap) and their analytical applications. 7. Mass spectrometry fragmentation and spectral interpretation Fragmentation mechanisms of molecular ions and interpretation rules in the structural analysis of organic compounds. 8. Applications of GC-MS and LC-MS in the analysis of complex samples Integration of chromatographic techniques with MS detection for the identification and quantitative analysis of multicomponent mixtures. 9. Nuclear magnetic resonance (NMR) physical principles, 1H and 13C NMR Principles of magnetic resonance, chemical shifts, spin-spin coupling, and interpretation of 1D NMR spectra. 10. NMR one- and two-dimensional spectra (COSY, HSQC, HMBC) Principles of correlation experiments and their application in determining the molecular framework of organic compounds. 11. NMR interpretation of spectra of organic compounds Structural analysis of selected organic compounds based on data from 1H, 13C, and 2D NMR spectra. 12. Complementarity of IR, Raman, NMR, MS and CD in structural analysis Strategies for integrating data from various spectroscopic techniques to unambiguously determine molecular structure. 13. Spectral databases SDBS, NIST, HMDB, PubChem Searching and interpreting spectral data using selected chemical and spectroscopic databases. 14. Applications of spectroscopy in chemical, pharmaceutical, and medical research Practical examples of using IR, Raman, NMR, MS, and CD in quality control, analysis of medicinal products, biologically active compounds, and related areas. 15. Spectroscopic identification strategy a systematic approach Planning measurements and making analytical decisions based on the interpretation of spectral data from multiple sources. **Laboratory** **I. Practical Fundamentals of UV-Vis, FTIR, and NMR Spectroscopy** 1. UV-Vis Spectroscopy introduction to the apparatus, spectrum recording, and qualitative analysis. Performing UV-Vis measurements for selected organic compounds with diverse structures, analysis of the absorption maxima, and the relationship between structure and spectrum (3h). Chromophoric systems: investigating the effect of the type and number of chromophore groups on the spectroscopic characteristics of an organic compound (3h). 2. FTIR Spectroscopy introduction to the apparatus, sample preparation in transmittance FTIR spectroscopy, spectrum recording. Reflectance methods in FTIR spectroscopy, comparison of transmittance and reflectance techniques (6h). 3. NMR Spectroscopy introduction to the apparatus, spectrum recording, spectrum interpretation. Analyzing the relationship between the structure of a series of selected organic compounds and the positioning of signals in proton (1H) and carbon (13C) nuclear magnetic resonance spectra (3h). **II. Practical Aspects of Spectral Interpretation Fundamentals of Structural Analysis** 1. Infrared Spectroscopy Basics of Spectrum Interpretation for Substances with Varying Structural Complexity, Substance Identification (3h) 2. Raman Spectroscopy Basics of Spectrum Interpretation for Substances with Varying Structural Complexity, Substance Identification (3h) 3. Nuclear Magnetic Resonance Spectroscopy (1H and 13C, 1D Spectra) Basics of Spectrum Interpretation for Substances with Varying Structural Complexity, Substance Identification (2h) 4. Nuclear Magnetic Resonance Spectroscopy (1H and 13C, 2D Spectra) Basics of Spectrum Interpretation for Substances with Varying Structural Complexity, Substance Identification (2h) 5. Mass Spectrometry Basics of Spectrum Interpretation for Substances with Varying Structural Complexity, Substance Identification (3h) 6. Integrated Structural Analysis Determining Structure Based on a Complete Set of Spectra (2h)
Prerequisites and co-requisites	Knowledge of the basics of organic chemistry.

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<tr><td>Assessment methods and criteria</td><td>

Subject passing criteria	Passing threshold	Percentage of the final grade
Written exam – theoretical fundamentals of spectroscopic methods and practical tasks (spectra interpretation)	51.0%	50.0%
Completion of practical exercises, passing short tests, preparation of reports	51.0%	25.0%
Problem solving – practical task: determination of the structure of a compound based on spectroscopic characteristics	51.0%	25.0%

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Recommended reading	Basic literature	1. R. M. Silverstein, F. X. Webster, D. J. Kiemle "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 2012. 2. "Spektroskopowe metody badania struktury związków organicznych", praca zbiorowa red. A. Rajca, WNT, Warszawa, 2000. 3. W. Danikiewicz Spektrometria mas, PWN, Warszawa, 2020. 4. L. K. Kazicyna, N. B. Kuplerska "Metody spektroskopowe wyznaczania struktury związków organicznych", PWN, Warszawa, 1974 5. R. A.W. Johnstone, M. E. Rose "Spektrometria mas podręcznik dla chemików i biochemików", PWN, Warszawa, 2001. 6. M. Gensicka-Kowalewska, M. J. Milewska, Podstawy metod badań struktury związków organicznych w zadaniach, Wydawnictwo PG, Gdańsk, 2024. 7. J. Twardowski, Spektroskopia Ramana i podczerwieni w biologii PWN, Warszawa, 1988.
	Supplementary literature	1. A. Zschunke "Spektroskopia magnetycznego rezonansu jądrowego w chemii organicznej", PWN Warszawa, 1976. 2. Z. Kęcki "Podstawy spektroskopii molekularnej", PWN, Warszawa, 2006.
	eResources addresses	
Example issues/ example questions/ tasks being completed	1. Based on the provided FTIR spectrum of the organic compound, identify the functional groups in the molecule. Determine the type of vibrations and assign characteristic peaks to the functional groups. 2. Using the data from the NMR spectrum (1H and 13C), determine the structure of the organic compound. Specify the number of protons, the position of the signals, and spin-spin couplings. Propose the structure of the compound. 3. In the provided mass spectrum, identify the molecular ion peak, the base peak, and the isotope peaks. Propose a possible structure of the compound based on the analysis of the spectrum. 4. Explain why FTIR spectroscopy and Raman spectroscopy are complementary techniques.	
Practical activites within the subject	Not applicable	