University of Gdańsk

Subject card

Subject name and code	Chemical spectroscopy, PG_00081981						
Field of study	Chemistry						
Date of commencement of studies	October 2024		Academic year of realisation of subject		2026/2027		
Education level	Bachelor's studies		Subject group		Obligatory subject group 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		2.0		
Learning profile	academic		Assessment form		exam		
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Sylwia Rodziewicz-Motowidło				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	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	15		2.0		33.0	50
Subject objectives	Introducing students to the physical principles of the interaction between electromagnetic radiation and matter, as well as the theoretical foundations of spectroscopic methods. The program includes knowledge acquisition in the fundamentals of mass spectrometry, vibrational spectroscopy (IR), and nuclear magnetic resonance spectroscopy (NMR) in 1D and 2D for ^{1}H-^{1}H and ^{13}C-^{1}H nuclei. Special emphasis will be placed on the practical applications of these techniques in chemical analysis, structural studies, and compound identification. The lectures will also focus on developing skills in spectrum interpretation, which is a key element in both laboratory and research work.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEML3_W04] Characterises the basic methods of chemical compound analysis.	The student can characterize spectroscopic methods used in the identification and analysis of chemical compounds. He knows their capabilities, limitations and applications in qualitative and quantitative analysis.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEML3_W07] Understands and describes physicochemical patterns, phenomena and processes using the language of mathematics.	The student understands the physical and mathematical principles underlying spectroscopy, including the phenomenon of magnetic resonance, molecular vibrations and ion fragmentation. He can apply mathematical models and relationships to describe spectra and their parameters.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEML3_U03] Selects the appropriate equipment and laboratory apparatus for conducting uncomplicated chemical experiments.	The student is able to select the appropriate spectroscopic technique and equipment for the type of chemical compound to be analyzed, taking into account the properties of the samples and the purpose of the study (identification, quantitative or structural analysis).	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written
[CHEML3_U02] Performs analyses using experimental methods and draws conclusions based on them.	The student is able to interpret spectroscopic results obtained by IR, NMR and MS techniques. On their basis, he formulates conclusions about the structure and properties of the analyzed chemical compounds.	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written
[CHEML3_W01] Enumerates basic laws and theories in chemistry, physics, mathematics and biology.	The student knows the basic physical and chemical laws underlying the operation of spectroscopic techniques (IR, NMR, MS), including the principle of magnetic resonance, molecular vibrations or ionization.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEML3_W03] Explains the relationship between the structure of matter and its observed properties.	The student understands how the structure of chemical molecules affects spectral parameters in IR, NMR and MS spectroscopy techniques. He can explain how changes in chemical structure lead to changes in the position, distribution and intensity of spectroscopic signals.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
[CHEML3_K03] Establishes priorities in the right way for the implementation of tasks specified by herself/himself and/or by others.	The student is able to determine the sequence of steps in the process of spectroscopic analysis of chemical compounds, taking into account the availability of apparatus, the properties of the samples and the research objectives.	[SK1] oral statement/conversation/ discussion [SK4] test/exam - oral or written
[CHEML3_U07] Prepares documented elaboration on a specific problem in the field of selected chemical and physical issues.	The student is able to prepare a written analysis of the results obtained by spectroscopic methods, using scientific literature, tables and experimental data.	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written

Subject contents

Properties of electromagnetic radiation and interaction of radiation with molecular systems: absorption, scattering, emission. Overview of MS, IR, 1D and 2D NMR techniques. 1D NMR spectra with 2D elements - COSY, TOCSY, HETCOR/HMQC, NOESY, DEPT etc; elements of spin systems analysis; identification of molecules with masses up to ~300 D; configuration, conformation, dynamics of molecules; emphasis on integrated application of spectroscopy methods for the most effective achievement of the mentioned goals; elements of conformational analysis of biomolecules.

Prerequisites and co-requisites

Passed basic organic chemistry and physical chemistry courses

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
exam	50.0%	100.0%

Recommended reading	Basic literature	-Collective edited by W. Zieliński and A. Rajca: Spectroscopic methods their application to the identification of organic compounds, WNT W-wa 1995, 2000.-R.M. Silverstein, F.X. Webster, D.J. Kiemle: Spectroscopic methods for the identification of organic compounds, PWN W-wa 2007 A.1.
	Supplementary literature	- A.S. Płaziak: Mass spectrometry of organic compounds, Wydaw. Naukowe UAM Poznań 1997- R.A.W. Johnstone, M.E. Rose: Mass spectrometry, PWN W-wa 2001.- Z. Kęcki: Fundamentals of Molecular Spectroscopy, PWN W-wa 1998.- I.Z. Siemion: Biostereochemistry, PWN Warsaw 1985.- K. Wüthrich: NMR in biological research: peptides and proteins, North-Holland, Amsterdam 1976.
	eResources addresses	
Example issues/ example questions/ tasks being completed	1. Explain the terms (formula, definition, unit): a) force constant, b) natural vibration, c) overtone, d) Fermi resonance.2. Explain how inductive and mesomeric effects affect the chemical shift of nuclei in 1H NMR spectroscopy.3. Calculate the number of degrees of freedom for a formaldehyde molecule (H2C=O) and then assign each of the degrees of freedom to a specific band of this molecule. Draw the IR spectrum of this molecule and mark on it the vibrations described earlier.	
Work placement	Not applicable	

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