



Subject card

Subject name and code	Methods of Structural Studies, PG_00053083						
Field of study	METODY BADAŃ STRUKTURALNYCH						
Date of commencement of studies	October 2023		Academic year of realisation of subject		2025/2026		
Education level	first-cycle studies		Subject group		Obligatory subject group in the field of study 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	6		ECTS credits		4.0		
Learning profile	general academic profile		Assessment form		exam		
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	30.0	0.0	0.0	0.0	30.0	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		5.0		35.0	100
Subject objectives	A main goal is to teach students basic spectroscopic methods including: NMR, IR, UV, and MS, and their application in the analysis of the structure of organic compounds						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	K6_W03		The student has knowledge of the theoretical foundations and applications of the most important spectroscopic methods; knows and understands the principle of operation and use of spectroscopy to identify chemical compounds		[SW1] Ocena wiedzy faktograficznej		
	K6_W02		knowledge connected with contemporary chemistry, containing properties and preparation methods of chemical compounds necessary for the calculations and for solving of spectral spectra		[SW3] Ocena wiedzy zawartej w opracowaniu tekstowym i projektowym		
	[K6_U01] knows how to get information from literature, databases and other sources, can integrate the information obtained, interpret and critically evaluate it, and draw conclusions, and to formulate and justify the opinions		The student uses the gained knowledge to obtain information on the structure of organic compounds		[SU1] Ocena realizacji zadania		

Subject contents	Course content – lecture Principles of spectroscopy electromagnetic radiation, energy levels in molecules, absorption of radiation, line shape, selection rules, application of the Fourier transformation in spectroscopy. 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, NOE, the Fourier transformation (FT-NMR), two-dimensional spectra (2D-NMR), basics of ¹⁹F and ¹³C NMR, elements of NMR of other nuclei. 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, the Raman spectroscopy. 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. Electronic spectra (UV-vis) electronic levels, spectrometers, selection rules, band shape, vibronic transitions, simple chromophores, aromatic chromophores, influence of substituents, steric effects, solvent effects. Course content – seminar Analysis and interpretation of ¹H and ¹³C NMR, IR, UV-vis, and MS spectra; Computer-assisted processing of the FID of the ¹H NMR spectrum											
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	<table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>teoretical colloquium</td><td>60.0%</td><td>50.0%</td></tr><tr><td>Midterm colloquium H and C NMR, IR, MS, UV</td><td>60.0%</td><td>50.0%</td></tr></table>			Subject passing criteria	Passing threshold	Percentage of the final grade	teoretical colloquium	60.0%	50.0%	Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%
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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, 2007. 2. "Spektroskopowe metody badania struktury związków organicznych", praca zbiorowa red. A. Rajca, WNT, Warszawa, 1996 lub 2000. 3. R. M. Silverstein, G. C. Bassler "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 1970. 4. L. K. Kazicyna, N. B. Kuplarska "Metody spektroskopowe wyznaczania struktury związków organicznych", PWN, Warszawa, 1974 5. M. Gensicka-Kowalewska, M.J. Milewska "Podstawy metod Badań Struktury Związków Organicznych w zadaniach" Wydawnictwo politechniki Gdańskiej, 2024 5. J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks "Organic Structural Spectroscopy' Prentice-Hall, Inc., 1998										

	Supplementary literature	1. R. A.W. Johnstone, M. E. Rose "Spektrometria mas podręcznik dla chemików i biochemików", PWN, Warszawa, 2001. 2. A. Zschunke "Spektroskopia magnetycznego rezonansu jądrowego w chemii organicznej", PWN Warszawa, 1976. 3. Z. Kęcki "Podstawy spektroskopii molekularnej", PWN, Warszawa, 1972. 4. H. Günther, "Spektroskopia magnetycznego rezonansu jądrowego", PWN, Warszawa, 1983.
	eResources addresses	Basic https://chem.pg.edu.pl/node/32/dla-studentow/chemia/metody-badan-strukturalnych - the lectures MJ Milewska http://www.irug.org/resources/spectral-databases-for-infrared - Spectral Databases for Infrared https://spectrabase.com/ - Online Spectral Database; Quick access to millions of NMR, IR, Raman, UV-Vis, and Mass Spectra.
Example issues/ example questions/ tasks being completed	1. The pair of protons at C-3 of cis-1,2-dichlorocyclopropane are diastereotopic. Explain. 2. Characterize the indicated protons as being homotopic, enantiotopic, or diastereotopic; magnetically equivalent or nonequivalent.. For example: 1-fluoro-1-iodoethene 3. Write out the rotamers of 2-chloroethanol. What is the spin notation at slow rotation for each rotamer and at fast rotation for the average?	
Practical activities within the subject	Not applicable	

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