



Subject card

Subject name and code	Methods for the structural study of substances - team project, PG_00060875						
Field of study	Metody badań strukturalnych substancji - projekt zespołowy						
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 Optional subject group		
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		2.0		
Learning profile	general academic profile		Assessment form		assessment		
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	15.0	0.0	0.0	15.0	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		3.0		17.0	50
Subject objectives	A main goal is to teach students basic spectroscopic methods including: NMR, IR, and MS, and their application in the analysis of the structure of organic compounds						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K6_U03] is able to apply knowledge of inorganic, organic, physical and analytical chemistry and identify appropriate sources of information to design and synthesize simple chemical compounds, carry out basic physicochemical and analytical measurements	Based on NMR and IR spectra, student can identify and point out functional groups present in organic compounds; student can introduce spectroscopic and slit-scan measurements and obtain computer-generated results.	[SU1] Ocena realizacji zadania
	[K6_U01] is able to acquire information from literature, databases and other appropriately selected sources, also in English; is able to integrate information obtained, interpret it and make conclusions, formulate and justify opinions	The student is able to use databases and software for processing spectroscopic data.	[SU4] Ocena umiejętności korzystania z metod i narzędzi
	[K6_K05] is aware of the social role of a technical university graduate, and in particular understands the need to formulate and communicate to the public, in particular through the mass media, information and opinions on the achievements of technology and other aspects of engineering activity	The student is able to communicate with specialists from other fields in a clear manner and provide information on issues related to simple spectroscopic studies.	[SK4] Ocena umiejętności komunikacji, w tym poprawności językowej
	[K6_W02] has knowledge of inorganic, organic, physical and analytical chemistry useful for obtaining selected groups of compounds, determining their physical and chemical properties allowing for their quantitative and qualitative analysis, making measurements and determining the parameters of chemical reactions, phenomena and processes occurring in chemical technology	Student is able to apply knowledge of the basics of physical, organic and inorganic chemistry and mathematics to analyze spectroscopic spectra.	[SW1] Ocena wiedzy faktograficznej

Subject contents	Course content – lecture 1. Principles of spectroscopy electromagnetic radiation, energy levels in molecules, absorption of radiation, line shape, selection rules, application of the Fourier transformation in spectroscopy. 2. 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, the Fourier transformation (FT-NMR), basics of ¹³C NMR. 3. 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. 4. 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. Course content – project Project Tasks Obligatory Tasks 1. Determining the chemical purity of the student preparation obtained during the organic synthesis labs: a) Measurement of ¹H NMR and IR spectra of an unknown sample b) Improvement of skills in the analysis and interpretation of ¹H and ¹³C NMR, IR, and MS spectra c) Computer-assisted processing of the FID of the ¹H NMR spectrum d) Analysis and interpretation of the obtained spectra e) Discussion of the purity and actual composition of the preparation from the student laboratory Elective Tasks 1. Design and conduct (with the assistance of an NMR operator) a spectroscopic experiment allowing for the observation of the ketone-enol equilibrium; analysis and interpretation of the obtained results, discussion of the effect of the solvent on the ketone-enol equilibrium, and determination of the ketone-enol concentration ratio. 2. Design and conduct (with the assistance of an NMR operator) a spectroscopic experiment predicting the exchange of protons for deuterons; analysis and interpretation of the obtained results, discussion of the effects of proton-deuteron exchange. 3. Design and conduct (with the assistance of an IR operator) a series of spectroscopic measurements on samples of common materials to detect compounds contained therein based on IR absorption by determining characteristic functional groups.		
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	Subject passing criteria	Passing threshold	Percentage of the final grade
	Reports on research conducted	100.0%	50.0%
	Midterm test NMR, IR, MS	60.0%	25.0%
	teoretical test	60.0%	25.0%
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. 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://spectrabase.com/ - Online Spectral Database; Quick access to millions of NMR, IR, Raman, UV-Vis, and Mass Spectra. http://www.irug.org/resources/spectral-databases-for-infrared - Spectral Databases for Infrared https://chem.pg.edu.pl/node/32/dla-studentow/chemia/metody-badan-strukturalnych - Selected topics from the lectures MJ Milewskiej
Example issues/ example questions/ tasks being completed	1. What characteristic of vibrational frequencies makes IR spectroscopy useful in determining structures of organic compounds? 2. How many kinds of nonequivalent protons are there in (a) p-diethylbenzene (b) 1,1,4-trichlorobutane? 3. Which electron is most likely to be lost in the ionization of the following compounds? (a) CH₄ (b) H₂C=CH₂ (c) H₂C=O	
Practical activities within the subject	Not applicable	

Document generated electronically. Does not require a seal or signature.