



Subject card

Subject name and code	Methods of structure elucidation, PG_00038530						
Field of study	Chemical Technology						
Date of commencement of studies	February 2023	Academic year of realisation of subject			2022/2023		
Education level	second-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	1	Language of instruction			Polish		
Semester of study	1	ECTS credits			3.0		
Learning profile	general academic profile	Assessment form			assessment		
Conducting unit	Department of Organic Chemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Maria Milewska					
	Teachers	prof. dr hab. inż. Maria Milewska prof. dr hab. inż. Dariusz Witt dr hab. Magdalena Śliwka-Kaszyńska dr hab. inż. Witold Przychodzeń dr inż. Karol Biernacki dr hab. Sławomir Makowiec					
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	15.0	0.0	0.0	45
	E-learning hours included: 0.0						
	Metody Badań Strukturalnych - Moodle ID: 29591 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=29591						
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	5.0		25.0	75	
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		
	K7_U01	Student is able to acquire information from literature, databases and other sources; is able to integrate the collected information, perform its interpretation and critical evaluation and also draw conclusions, formulate and extensively validate the opinions			[SU1] Assessment of task fulfilment		
	K7_U04	Student recognizes the functional groups present in organic compounds upon interpretation of IR spectra; interprets NMR, IR and MS spectra, is able to describe NMR, IR, MS and UV-vis spectra; identifies organic compounds on the basis of NMR, IR, MS and UV-vis spectra			[SU4] Assessment of ability to use methods and tools		

Subject contents	<p>Principles of spectroscopy – electromagnetic radiation, energy levels in molecules, absorption of radiation, line shape, selection rules, application of the Fourier transformation in spectroscopy.</p> <p>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.</p> <p>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.</p> <p>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.</p> <p>Electronic spectra (UV-vis) – electronic levels, spectrometers, selection rules, band shape, vibronic transitions, simple chromophores, aromatic chromophores, influence of substituents, steric effects, solvent effects.</p>											
Prerequisites and co-requisites	<ol style="list-style-type: none"> 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 border="1"> <thead> <tr> <th data-bbox="456 1279 794 1308">Subject passing criteria</th> <th data-bbox="799 1279 1137 1308">Passing threshold</th> <th data-bbox="1142 1279 1481 1308">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="456 1314 794 1341">theoretical colloquium</td> <td data-bbox="799 1314 1137 1341">60.0%</td> <td data-bbox="1142 1314 1481 1341">50.0%</td> </tr> <tr> <td data-bbox="456 1348 794 1388">Midterm colloquium H and C NMR, IR, MS, UV</td> <td data-bbox="799 1348 1137 1388">60.0%</td> <td data-bbox="1142 1348 1481 1388">50.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	theoretical colloquium	60.0%	50.0%	Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%
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Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%										
Recommended reading	Basic literature	<ol style="list-style-type: none"> 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. J. Milewska, Wykłady, http://www.pg.gda.pl/chem/Katedry/Organa/dydaktyka.htm 										

	Supplementary literature	<p>1. R. A.W. Johnstone, M. E. Rose "Spektrometria mas – podręcznik dla chemików i biochemików", PWN, Warszawa, 2001.</p> <p>2. A. Zschunke "Spektroskopia magnetycznego rezonansu jądrowego w chemii organicznej", PWN Warszawa, 1976.</p> <p>3. Z. Kęcki "Podstawy spektroskopii molekularnej", PWN, Warszawa, 1972.</p> <p>4. H. Günther, "Spektroskopia magnetycznego rezonansu jądrowego", PWN, Warszawa, 1983.</p> <p>5. M. Szafran, Z. Dega-Szafran "Określenie struktury związków organicznych metodami spektroskopowymi", PWN, Warszawa, 1988</p>
Example issues/ example questions/ tasks being completed	eResources addresses	
Work placement	Not applicable	