GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Methods of structure elucidation, PG_00066879		
Field of study	Chemical Technology		
Date of commencement of studies	February 2025	Academic year of realisation of subject	2024/2025
Education level	second-cycle studies	Subject group	
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	exam
Conducting unit	Department of Organic Chemistry -> Faculty of Chemistry -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Sławomir Makowiec	
	Teachers		

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

eNauczanie source addresses:

Moodle ID: 45802 Metody Badań Strukturalnych
https://enauczanie.pg.edu.pl/moodle/course/view.php?id=45802

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	0.0	0.0	45

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_W06] integrates knowledge from different disciplines, principles of intellectual property protection and patent law, relevant for appropriate interpretation and application in scientific, sustainable economic activities	The student knows how to apply the acquired information in the field of various spectroscopic techniques.	[SW1] Assessment of factual knowledge
[K7_W02] selects appropriate apparatus and materials for the manufacture and processing of consumer goods	The student knows what spectroscopic technique to use to determine the structure of a molecule.	[SW1] Assessment of factual knowledge
[K7_U01] designs experiments using computer methods of data analysis, computer simulations and based on the state of the knowledge in accordance with the latest scientific literature	The student is able to select the appropriate spectroscopic technique to monitor a process or to determine the structure of a molecule.	[SU2] Assessment of ability to analyse information
[K7_U04] predicts the properties of the materials obtained and the course of processes involving them, based on knowledge of technology and related fields and computer methods of data analysis, modelling and simulation	The student is able to predict what the spectrum of a molecule should look like in a given spectroscopic techniqu	[SU1] Assessment of task fulfilment

Subject contents	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.
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
teoretical colloquium	60.0%	50.0%
Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%

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. L. K. Kazicyna, N. B. Kuplerska "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	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. 5. M. Szafran, Z. Dega-Szafran "Określenie struktury związków organicznych metodami spektroskopowymi", PWN, Warszawa, 1988
	eResources addresses	
Example issues/ example questions/ tasks being completed		
Work placement	Not applicable	

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