GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Methods of structure elucidation, PG_00038530		
Field of study	Chemical Technology		
Date of commencement of studies	February 2024	Academic year of realisation of subject	2023/2024
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 dr hab. inż. Witold Przychodzeń	

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						

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_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
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

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
Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%
teoretical colloquium	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	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed		
Work placement	Not applicable	