GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Methods of structural studies, PG_00057707		
Field of study	Green Technologies		
Date of commencement of studies	October 2022	Academic year of realisation of subject	2024/2025
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	5	ECTS credits	2.0
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	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	15.0	0.0	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	2.0	18.0	50

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_U03] is able to use information and communication technologies relevant to the common tasks of engineering, is able to use known methods and mathematical-physical models to describe and explain phenomena and chemical processes	The student knows how to use databases and software for processing spectroscopic data.	[SU4] Assessment of ability to use methods and tools
[K6_W01] has a basic knowledge from some branches of mathematics and physics useful for formulating and solving simple problems in the field of environmental technologies and modern analytical methods	The student knows the physical basis of IR, NMR and MS spectroscopy. The student has knowledge of the basics of spectroscopic methods; knows and understands the principle of operation and application of the most important spectroscopic methods to analyze the structure of organic compounds	[SW1] Assessment of factual knowledge
[K6_W02] has a basic knowledge of chemistry including general chemistry, inorganic, organic, physical, analytical, including the knowledge necessary to describe and understand the phenomena and chemical processes occurring in the environment; measurement and the determination of the parameters of these processes.	Student is able to apply knowledge of the basics of physical, organic and inorganic chemistry and mathematics to analyze spectroscopic spectra.	[SW1] Assessment of factual knowledge

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, the Fourier transformation (FT-NMR), two-dimensional spectra (2D-NMR), basics of ^{19}F and ^{13}C NMR, elements of NMR. 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 tests 1H and 13C NMR, IR, MS, UV	60.0%	50.0%
teoretical test	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. J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks "Organic Structural Spectroscopy' Prentice-Hall, Inc., 1998

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. Gensicka-Kowalewska, M. J. Milewska"Podstawy metod Badania Struktury Związków Organicznych w zadaniach" , Wydawnictwo PG, Gdańsk, 2024
	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	1. What characteristic of vibrational frequencies makes IR spectroscopyuseful 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 in most like to be lost in the ionization of the following compounds? (a) CH_4 (b) $H_2C=CH_2$ (c) $H_2C=O$	
Work placement	Not applicable	