GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Methods of Structural Studies, PG_00036275		
Field of study	Green Technologies		
Date of commencement of studies	October 2021	Academic year of realisation of subject	2022/2023
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	2	Language of instruction	Polish
Semester of study	4	ECTS credits	4.0
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	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	30.0	0.0	0.0	60

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	60	5.0	35.0	100

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	Student is able to analyze the IR, NMR, MS spectra and assign the appropriate structural formula of the compound.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools
[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.	The student knows the physical basis of IR, NMR and MS spectroscopy.	[SW1] Assessment of factual knowledge
[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.	[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, 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 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. 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	