GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Methods of Structural Studies, PG_00053083		
Field of study	Chemistry		
Date of commencement of studies	October 2021	Academic year of realisation of subject	2023/2024
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	6	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	exam
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. Teresa Olszewska dr inż. Karol Biernacki	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	0.0	0.0	30.0	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_W02	knowledge connected with contemporary chemistry, containing properties and preparation methods of chemical compounds necessary for the calculations and for solving of spectral spectra	[SW3] Assessment of knowledge contained in written work and projects
[K6_U01] knows how to get information from literature, databases and other sources, can integrate the information obtained, interpret and critically evaluate it, and draw conclusions, and to formulate and justify the opinions	The student uses the gained knowledge to obtain information on the structure of organic compounds	[SU1] Assessment of task fulfilment
K6_W03	The student has knowledge of the theoretical foundations and applications of the most important spectroscopic methods; knows and understands the principle of operation and use of spectroscopy to identify chemical compounds	[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 ^{19}F and ^{13}C 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. J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks "Organic Structural Spectroscopy' Prentice-Hall, Inc., 1998
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.

	eResources addresses	Adresy na platformie eNauczanie: 2023/2024 Metody Badań Strukturalnych CHEMIA - Moodle ID: 38111 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=38111
Example issues/ example questions/ tasks being completed	1. The pair of protons at C-3 of cis-1,2-dichlorocyclopropane are diastereotopic. Explain. 2. Characterize the indicated protons as being homotopic, enantiotopic, or diastereotopic ; magnetically equivalent or nonequivalent.. For example: 1-fluoro-1-iodoethene 3. Write out the rotamers of 2-chloroethanol. What is the spin notation at alow ratiation for each rotamer and at fast ratation for the average?	
Work placement	Not applicable	

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