GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	METHODS OF STRUCTURAL STUDIES, PG_00064409						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject	2028/2029			
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	assessment			
Conducting unit	Department of Organic Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. inż. Maria Milewska				
	Teachers						
Lesson types	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	The aim of the course is to teach students how to interpret spectra by leveraging the synergistic information provided by NMR, IR, and electronic spectroscopy, as well as mass spectrometry. These spectroscopic techniques utilize electromagnetic radiation of varying energies, with the resulting spectra representing the sample compound's response to the applied radiation. The lectures will cover: (1) the theoretical principles and acquisition methods for infrared spectra; (2) the fundamentals of nuclear magnetic resonance (NMR), including proton, carbon, and fluorine resonance; (3) the theoretical basis of electronic transitions; and (4) molecular ionization methods and the fragmentation pathways of ionized compounds. Laboratory sessions will focus on methods for identifying the structures of chemical compounds based on spectroscopic and mass spectra.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U07] is able to undertake accurate and precise analytical measurements, to synthesise simple and large-molecular chemical compounds, to purify and analyse their composition and to determine their structure using classical and instrumental methods	is able to determine the structure of organic compounds using spectroscopic methods and mass spectra.	[SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools
[K6_U01] gathers information from literature, databases and other sources, interpreting, critically evaluating, summarising, formulating and justifying opinions, independently analyses and produces technical drawings with the use of computer assistance	applies the knowledge to obtain information on the relationship between the spectroscopic spectra and the chemical structure of organic compounds.	[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject
[K6_K03] is aware of the importance of caring for the quality and diligence of the tasks performed, being responsible for their consequences	is prepared to conduct a careful analysis of spectroscopic spectra.	[SK2] Assessment of progress of work
[K6_W02] classifies acquired information, assessing its usefulness in solving the posed problems concerning the synthesis and analysis of selected groups of compounds, determining their physical and chemical properties, making measurements and determining the parameters of chemical reactions and processes	possesses organized, theoretically grounded general knowledge connected with contemporary chemistry, containing properties and preparation methods of chemical compounds necessary for the calculations and for solving of spectroscopic spectra	[SW1] Assessment of factual knowledge

Subject contents

Course content – lecture

Principles of spectroscopy – electromagnetic radiation, energy levels in molecules, absorption of radiation, line shape, selection rules, application of the Fourier transformation in spectroscopy.

NMR spectroscopy – magnetic properties of atomic nuclei, the chemical shift, the spin-spin coupling, diamagnetic anisotropy of molecules, 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.

Infrared spectroscopy (IR) – harmonic and anharmonic oscillator, vibrations of multiatom molecules, the normal vibrations, transition probability, group frequencies, 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.

Course content – laboratory

The aim of the course is to acquire the skills to determine the structure of organic compounds based on spectra obtained via NMR, IR, and UV-Vis spectroscopy and mass spectrometry:

- interpretation of the proton and carbon NMR spectra
- measurements of the IR spectra; interpretation of the IR spectra
- interpretation of mass spectra – determination of molecular mass; description of ion fragmentation

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

<table>
<tr><td>Assessment methods and criteria</td><td colspan="2"><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Lecture: teoretical colloquium</td><td>60.0%</td><td>50.0%</td></tr>
<tr><td>Laboratory: midterm colloquium H and C NMR, IR, MS, UV</td><td>60.0%</td><td>50.0%</td></tr>
</table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td>1. R. M. Silverstein, F. X. Webster, D. J. Kiemle "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 2012.
2. "Spektroskopowe metody badania struktury związków organicznych", praca zbiorowa red. A. Rajca, WNT, Warszawa, 1996 lub 2000.
3. J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks "Organic Structural Spectroscopy' Prentice-Hall, Inc., 1998</td></tr>
<tr><td>Supplementary literature</td><td>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. Z. Głowacki "Podstawy spektroskopowych metod badania struktury związków organicznych. Wademekum wraz z zadaniami" Tutor, 2022.
6. M. Gensicka-Kowalewska, M. J. Milewska "Podstawy metod badań struktury związków organicznych w zadaniach" , Wydawnictwo PG, Gdańsk, 2024.</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="2">1. Characterize the indicated protons as being homotopic, enantiotopic, or diastereotopic ; magnetically equivalent or nonequivalent.. For example: 1-fluoro-1-iodoethene

2. Write out the rotamers of 2-chloroethanol. What is the spin notation at alow rotiation for each rotamer and at fast rotation for the average?</td></tr>
<tr><td>Practical activites within the subject</td><td colspan="2">Not applicable</td></tr>
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