GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Methods for the structural study of substances - team project, PG_00060875		
Field of study	Chemical Technology		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2027/2028
Education level	first-cycle studies	Subject group	Obligatory subject group in the field of study Optional subject group
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	2.0
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	15.0	0.0	0.0	15.0	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	3.0	17.0	50

Subject objectives

A main goal is to teach students basic spectroscopic methods including: NMR, IR, and MS, and their application in the analysis of the structure of organic compounds

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U01] Is able to independently plan the learning process and acquire, analyse and interpret information from various sources, also in English.	is able to use databases and software for processing spectroscopic data.	[SU4] Assessment of ability to use methods and tools
[K6_W02] Possesses the chemical knowledge necessary to synthesize, analyze and evaluate the properties of compounds and processes used in chemical technology.	has theoretical knowledge of the fundamentals of physical, organic, and inorganic chemistry, as well as mathematics for the analysis of spectroscopic spectra.	[SW1] Assessment of factual knowledge
[K6_U03] Uses chemical knowledge to design compounds, perform physicochemical and analytical measurements, and obtain appropriate sources of information.	is able to recognize and identify functional groups present in the structure of organic compounds based on NMR and IR spectra; the student is able to perform spectroscopic measurements and process the obtained results using a computer	[SU1] Assessment of task fulfilment

Subject contents

Course content – lecture

1. Principles of spectroscopy electromagnetic radiation, energy levels in molecules, absorption of radiation, line shape, selection rules, application of the Fourier transformation in spectroscopy.
2. 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), basics of ^{13}C NMR.
3. 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.
4. 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.

Course content – project

Project Tasks

Obligatory Tasks

1. Determining the chemical purity of the student preparation obtained during the organic synthesis labs:

a) Measurement of ^{1}H NMR and IR spectra of an unknown sample

b) Improvement of skills in the analysis and interpretation of ^{1}H and ^{13}C NMR, IR, and MS spectra

c) Computer-assisted processing of the FID of the ^{1}H NMR spectrum

d) Analysis and interpretation of the obtained spectra

e) Discussion of the purity and actual composition of the preparation from the student laboratory

Elective Tasks

1. Design and conduct (with the assistance of an NMR operator) a spectroscopic experiment allowing for the observation of the ketone-enol equilibrium; analysis and interpretation of the obtained results, discussion of the effect of the solvent on the ketone-enol equilibrium, and determination of the ketone-enol concentration ratio.

2. Design and conduct (with the assistance of an NMR operator) a spectroscopic experiment predicting the exchange of protons for deuterons; analysis and interpretation of the obtained results, discussion of the effects of proton-deuteron exchange.

3. Design and conduct (with the assistance of an IR operator) a series of spectroscopic measurements on samples of common materials to detect compounds contained therein based on IR absorption by determining characteristic functional groups.

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 test NMR, IR, MS	60.0%	25.0%
Reports on research conducted	100.0%	50.0%
teoretical test	60.0%	25.0%

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

	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	
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) $H_2C=O$	
Practical activites within the subject	Not applicable	

Document generated electronically. Does not require a seal or signature.