University of Gdańsk

Subject card

Subject name and code	Spectrochemistry, PG_00117689		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
Education level	postgraduate studies	Subject group	Obligatory subject group in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish polish
Semester of study	2	ECTS credits	2.0
Learning profile	academic	Assessment form	
Conducting unit	Pracownia Chemii Medycznej -> Katedra Chemii Biomedycznej -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Emilia Sikorska	
	Teachers	dr hab. Emilia Sikorska	

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	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	15	2.0	33.0	50

Subject objectives	Practical application of spectroscopic methods; consolidation of the knowledge on mass spectrometry, IR and NMR spectroscopy; basics of Raman spectroscopy, spectrofluorimetry, optical rotatory dispersion and circular dichroism and their elementary applications; deepening of knowledge about 1D and 2D NMR to the extent necessary for spectra interpretation of compounds up to ~300 D; learning to interpret the spectra to determine the structure (hydrogen bonds, stereochemistry, dynamics etc.) including the advantages and disadvantages of the methods; introduction to the analysis of biomolecules.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_K02] Works in a team taking on various roles in it.	Student follows safety procedures in laboratory work; works in a team (leader / group relationship); mobilizes and motivates group members to work; takes responsibility for the actions taken.	[SK5] implementation of a problem task [SK6] demonstration of practical skills [SK8] observation of student's independent or team work
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Student appreciates the need for continuous education in the" information" society of the 21st century; shows creativity, criticism in using the Internet; complies with the principles of ethics and copyright.	[SK1] oral statement/conversation/ discussion [SK5] implementation of a problem task [SK8] observation of student's independent or team work
[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.	Student appreciates the need for continuous education in the" information" society of the 21st century; shows creativity, criticism in using the Internet; complies with the principles of ethics and copyright.	[SU1] oral statement/conversation/ discussion [SU4] test/exam - oral or written [SU5] implementation of a problem task
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student knows the mathematical and physical basis of various spectroscopic methods; is able to qualitatively and quantitatively analyze spectroscopic data.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
[CHEMMU2_W03] Demonstrates extended knowledge in the field of modern measuring techniques used in chemical analysis.	Student knows and understands the theoretical basis of various molecular spectroscopy methods with their advantages and disadvantages; is able to use spectroscopy methods to analyze the structure and properties of organic compounds; characterizes and distinguishes selected aspects of structure and interactions, such as topology, geometric and optical isomerization, tautomerism, and hydrogen bonds; knows the basic aspects of the construction and operation of measuring devices; has the knowledge to quantitative description of chemical phenomena and processes.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
[CHEMMU2_W02] Has extended and in-depth knowledge in the field of basic chemistry.	Student knows and understands the theoretical basis of organic and physical chemistry; characterizes and distinguishes selected aspects of structure and interactions, such as topology, geometric and optical isomerization, tautomerism, and hydrogen bonds; has the knowledge to quantitative description of chemical phenomena and processes.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	Student uses specialized software to analyze spectroscopic data.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	Student knows and understands the theoretical basis of various molecular spectroscopy methods with their advantages and disadvantages; is able to use spectroscopy methods to analyze the structure and properties of organic compounds; knows the basic aspects of the construction and operation of measuring devices; has the knowledge to quantitative description of chemical phenomena and processes.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task

Subject contents	Short overview of techniques: MS, IR, and NMR necessary for solving structures of organic compounds with reference to the Spectroscopy course at the first-degree studies; UV/VIS spectrophotometry, Raman spectroscopy, fluorescence spectroscopy and spectrofluorimetry; circular dichroism; multidimensional NMR spectroscopy; analysis of spin systems (AB-AX, ABC-AMX, AA'BB'-AA'XX', etc); identification of molecules up to ~300 Da; configuration, conformation and dynamic of the molecules; elements of conformational analysis of biomolecules; integrated use of the spectroscopic methods for the most effective achievement of the goals.
Prerequisites and co-requisites	Passed the basic course in organic chemistry and chemical spectroscopy at the 1st degree in the field of Chemistry

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
written exam with open questions	51.0%	15.0%
written exam (test)	51.0%	85.0%

Recommended reading

Basic literature	1. Collectively edited W. Zieliński i A. Rajca: Metody spektroskopowe ich zastosowanie do identyfikacji związków organicz-nych, WNT W-wa 1995, 2000. 2. R.M. Silverstein, F.X. Webster, D.J. Kiemle: Spektroskopowe metody identyfikacji związków organicznych, PWN W-wa 2007 3. B. Wojtkowiak, Martial Chabanel: Spektroskopia molekularna, PWN W-wa 1984. 4. Z. Kęcki: Podstawy spektroskopii molekularnej, PWN Warszawa 1998. 5. W. Danikiewicz: Spektrometria mas: Podstawy i zastosowania, PWN W-wa 2020
Supplementary literature	1. H. Barańska, A. Łabudzińska, J. Terpiński: Laserowa spektrometria ramanowska, zastosowania analityczne, 1981, PWN, Warszawa, 2. A. S. Płaziak: Spektrometria masowa związków organicznych, Wydaw. Naukowe UAM Poznań 1997 3. R.A.W. Johnstone, M.E. Rose: Spektrometria mas, PWN W-wa 2001 4. H. Barańska, A. Łabudzińska, J. Terpiński: Laserowa spektrometria Ramanowska, zastosowania analityczne, PWN, Warszawa 1981. 5. S. Paszyc. Podstawy fotochemii, PWN Warszawa 1992 6. I.Z. Siemion: Biostereochemia, PWN Warszawa 1985. 7. K. Wüthrich: NMR in biological research: peptides and proteins, North-Holland, Amsterdam 1976.Internet: poszukiwania samodzielne, weryfikowane przez prowadzącego zajęcia.
eResources addresses	Podstawowe https://www.nmrdb.org/ - Online program enabling simulation of NMR spectra (available on 13.06.2024). Adresy na platformie eNauczanie:

Example issues/ example questions/ tasks being completed	
Work placement	Not applicable

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