UNIWERSYTET GDAŃSKI

Course title
Spektrochemia/Spectrochemistry

ECTS code
13.3.0849

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemistry	Master	Full-time studies	

Teaching staff
dr hab. Emilia Sikorska, prof. UG; Sylwia Rodziewicz-Motowidło, prof. UG; dr hab. Zbigniew Kaczyński, prof. UG; dr Małgorzata Czerwicka-Pach; dr Marta Spodzieja

Forms of classes, the realization and number of hours

A. Forms of classes, in accordance with the UG Rector's regulations
lecture, laboratory classes

B. The realization of activities
In-class learning

Number of hours
lecture 15 h, laboratory classes 30 h

ECTS credits
classes 45 h
Tutorial classes 10 h
Student's own work 45 h
TOTAL: 100 h - 4 ECTS

The academic cycle
First year, summer semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods
- Laboratory experiments
- designing chemical experiments
- Lectures including multimodal presentations
- Case studies

Form and method of assessment and basic criteria for evaluation or examination requirements

A. Final evaluation, in accordance with the UG study regulations
Course completion (with a grade), exam

B. Assessment methods
- Laboratory exercises: the final grade determined based on partial grades (tests and written reports) obtained during the semester.
- Lecture: test containing up to 20 questions, including up to 3 spectra with medium degree of difficulty

C. The basic criteria for evaluation or exam requirements

Individual and/or team work on research tasks; positive grades from tests and written reports from laboratory exercises; the final grade will be determined based on the partial grades (arithmetic average); failure to execute the laboratory exercises means failure to achieve a pass. A student who has completed laboratory exercises with the positive grade can take the exam.

Required courses and introductory requirements
Organic and physical chemistry

Aims of education
Practical application of spectroscopic methods; consolidation of the knowledge on mass spectrometry, oscillation spectroscopy (IR) and nuclear magnetic resonance NMR spectroscopy; basics of Raman spectroscopy, fluorescence spectroscopy and spectrofluorimetry, optical rotatory dispersion and circular

dichroism and their elementary applications; deepening of knowledge about 1D and 2D NMR spectroscopy to the extent necessary for spectra interpretation of compounds up to ~300 D; familiarize the students with the use of spectroscopic methods in identification of topology of compounds, hydrogen bonds, stereochemistry, dynamics etc. including the advantages and disadvantages of the methods; introduction to the analysis of biomolecules.

Course contents

A. Lecture: 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.

B. Laboratory exercises: The basics of spectroscopic methods; methodology; apparatus construction; advantages and disadvantages of the spectroscopic methods. Measurements and analysis of MS, IR, NMR, UV/VIS spectra. Practical aspect of spectroscopic methods for conformational and dynamic studies of molecules up to ~300 D. Analysis of intra- and intermolecular interactions. Study of the effect of concentration, solvent, temperature on the spectra. Dynamic effects in the NMR spectroscopy. Elements of analysis of the structure and conformation of biomolecules.

Bibliography of literature

A. Literature required to pass the course

-Zbiorowa pod red. W. Zieliński i A. Rajca: Metody spektroskopowe ich zastosowanie do identyfikacji związków organicz-nych, WNT W-wa 1995, 2000.
-R.M. Silverstein, F.X. Webster, D.J. Kiemle: Spektroskopowe metody identyfikacji związków organicznych, PWN W-wa 2007
-H. Barańska, A. Łabudzińska, J. Terpiński: Laserowa spektrometria ramanowska, zastosowania analityczne, 1981, PWN, Warszawa,

A.1. literaturę used during classes:

- Internet: information found by the student and verified by the teacher.
-B. Wojtkowiak, Martial Chabanel: Spektroskopia molekularna, PWN W-wa 1984.

B. Extracurricular readings

-A. S. Płaziak: Spektrometria masowa związków organicznych, Wydaw. Naukowe UAM Poznań 1997
- R.A.W. Johnstone, M.E. Rose: Spektrometria mas, PWN W-wa 2001
-Z. Kęcki: Podstawy spektroskopii molekularnej, PWN Warszawa 1998.
-H. Barańska, A. Łabudzińska, J. Terpiński: Laserowa spektrometria ramanowska, zastosowania analityczne, PWN, War-szawa 1981.
-S. Paszyc. Podstawy fotochemii, PWN Warszawa 1992
-I.Z. Siemion: Biostereochemia, PWN Warszawa 1985.
-K. Wüthrich: NMR in biological research: peptides and proteins, North-Holland, Amsterdam 1976.

Knowledge

Student knows and understands the theoretical basis for various molecular spectroscopy with their advantages and disadvantages. Student 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.
Skills Student plans and / or performs measurements; interprets the results; presents the results in the form of a written report.
Social competence 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; follows safety procedures in laboratory work; works in a team (leader / group relationship).