UNIWERSYTET GDAŃSKI

Course title
Spektroskopia chemiczna / Chemical spectroscopy

ECTS code
13.3.0727

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemical Business	Bachelor / Engineer	Full-time studies	

Teaching staff
prof. Sylwia Rodziewicz-Motowidło, dr hab. Emilia Sikorska, prof. Zbigniew Kaczyński

Forms of classes, the realization and number of hours

A. Forms of classes, in accordance with the UG Rector's regulations
lectures, auditorium classes

B. The realization of activities
multimedia presentation, in-class learning

C. Number of hours
45 h (15 h lecture, 30 h auditorium classes)

ECTS credits 4

classes - 45 h
tutorial classes – 10 h
student's own work – 45 h

Total: 100 h - 4 ECTS

The academic cycle
2021/22 winter semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods

- Lecture with multimedia presentation,
- In the auditorium classes students will learn combined interpretation of the mass, IR, ^{1}H and ^{13}C NMR spectra of compounds of M.W. up to ~300 D by solving problems designated by the teacher (in-class on the board and in a group-/home-work.

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

A. Final evaluation, in accordance with the UG study regulations
lectures - exam,
auditorium classes – course credit with a grade

B. Assessment methods
Lecture

- written exam, 5-10 tasks to solve, including spectra with medium degree of difficulty

Auditorium classes

- 4-5 obligatory 10 minutes tests from previously trained material
- current knowledge control based on spectroscopic problems previously given for practice by the teacher
- quizzes on the fastest correct solution of spectroscopic problems given by the teacher during seminars

C. The basic criteria for evaluation or exam requirements

Lecture:
• pass the written exam
91-100%: 5.0
81-90%: 4.5
71-80%: 4.0
61-70%: 3.5
51-60%: 3.0
Less than 51% 2.0

Auditorium classes:
• completed all tests, additional problems and quizzes
91-100%: 5.0
81-90%: 4.5
71-80%: 4.0
61-70%: 3.5

	51-60%: 3.0 Less than 51% 2.0
	D. Method of verification of the established effects of education Lecture: • A written exam consisting of 5-10 problems covering the topics presented during the lecture and auditorium classes. Passed classes tests (see below) is prerequisite. • Attendance at lectures are not obligatory (although presence is recommended), and the lack of knowledge resulting from the absence may be made up on the basis of other students' notes and literature. Auditorium classes: • Attendance, active participation, completed tests.

Required courses and introductory requirements
Organic and physical chemistry

Aims of education

- Presenting the physical basics of the interactions of electromagnetic radiation with matter and the theoretical basis of spectroscopic methods to students
- Familiarize the students with the fundamentals of mass spectrometry (MS), oscillation spectroscopy (IR) and 1D and 2D nuclear magnetic resonance (NMR) spectroscopy;
- Familiarize the students with interpretation of MS, IR and NMR spectra of compounds up to ~ 300 D to identify the topology, hydrogen bonds, stereochemistry, dynamics etc. including the advantages and disadvantages of the used methods.

Course contents

A. Topics of the lecture: The properties of the electromagnetic radiation and its interactions with molecular systems: absorption, emission, dispersion. Overview of techniques: MS, IR, and NMR, including 2D NMR methods such as: COSY, TOCSY, HSQC/HMQC, NOESY; spin systems analysis, identification of molecules up to ~ 300 D; configuration, conformation, dynamic of the molecules; integrated usage of the spectroscopic methods; elements of conformational analysis of biomolecules.

B. Auditorium classes: Interpretation of the spectra; practical use of spectroscopic methods in structural and dynamics studies of molecules up to ~300D; to familiarize of the students with the probability of several different solutions of the same problem and verification of the correct solution; learning of the correct description of the spectra; to know the disadvantages and advantages of the particular spectroscopic methods, complementarity of the spectroscopic methods.

Bibliography of literature

A. Literature required to pass the course

- Collective red.. W. Zieliński i A. Rajca: Metody spektroskopowe ich zastosowanie do identyfikacji związków organicznych, WNT W-wa 1995, 2000.
- R.M. Silverstein, F.X. Webster, D.J. Kiemle: Spectrometric Identification of Organic Compounds, John Wiley & Sons, 2005, 2014.
- Internet: independent study, verified by the teacher.

B. Extracurricular readings

- S. Płaziak: Spektrometria masowa związków organicznych, Wydaw. Naukowe UAM Poznań 1997
- R.A.W. Johnstone, M.E. Rose: Mass spectrometry for chemists and biochemists. Cambridge University, 1982, 1996
- Z. Kęcki: Podstawy spektroskopii molekularnej, PWN Warszawa 1998.
- I.Z. Siemion: Biostereochemia, PWN Warszawa 1985.
- K. Wüthrich: NMR in biological research: peptides and proteins, North-Holland, Amsterdam 1976.

Knowledge

Students know theoretical basis for spectroscopic methods utilized in identification of simple organic compounds
Students know the advantages and disadvantages of spectroscopic methods
Students have basic knowledge about conformational analysis of biomolecules using spectroscopic methods
Students can present the current trends in the development of spectroscopic methods

Skills

Students are able to interpret MS, IR, NMR spectra of simple organic compounds,
Students have skills of drawing correct conclusions based on available data.

Social competence

Individually and/or in a team-work:

-Students can establish and realize a defined action plan setting priorities for its implementation.

-Students can identify their level of knowledge and skills and understand the necessity of life-long learning in chemical spectroscopy and personal development.

Contact

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