

**DOCTORAL SCHOOL OF WROCLAW UNIVERSITY OF SCIENCE AND
TECHNOLOGY**

SUPERVISOR/TEAM/ DECLARING/CONDUCTING COURSE: Wojciech Bartkowiak
DEPARTMENT W-03 / K-17

COURSE CARD

Course name in Polish: Spektroskopia Molekularna

Course name in English: Molecular Spectroscopy

Course language Polish / ~~English~~*

Specialized courses for PhD students receiving education in discipline:* interdisciplinary course in the field of several disciplines: theoretical chemistry and physics

Subject code: NCQ100172W

* delete as applicable

	Lecture	Foreign language course	Seminar	Mixed forms
Number of hours of organized classes in university (ZZU)	30	-	-	-
Grading	Exam	-	-	-
Number of ECTS points				

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General chemistry and physics
2. Linear algebra and mathematical analysis
3. Basics of physical chemistry with elements of quantum chemistry or solid state physics

COURSE OBJECTIVES

- C1. To provide students with a general knowledge regarding light-matter interactions.
- C2. To provide students with a ability to interpret absorption and emission spectra of molecules.
- C3. To acquaint students with a review of applications of spectroscopic techniques in studies of molecular structures at various levels of complexity.

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PROGRAM CONTENTS

Form of classes – lecture (Lec)		Number of hours
Lec1	Development of atomic and molecular spectroscopy – a historical perspective.	2
Lec2	Basic concepts related to spectroscopy. Structure of absorption and emission spectra. Broadening mechanisms of bands in atomic and molecular spectra.	2
Lec3	Lambert-Beer law. Transition intensities.	2
Lec4	Basics of quantum mechanics. Time-dependent Schrodinger equation.	2
Lec5	Quantum-mechanical description of light-matter interactions. Time-dependent perturbation theory.	2
Lec6	Selection rules in molecular spectroscopy.	2
Lec7	Spectrum of molecular rotational states. Microwave spectroscopy.	2
Lec8	Spectrum of molecular vibrational states. Infra red spectroscopy.	2
Lec9	Introduction to electronic energy levels of atoms and molecules.	2
Lec10	Jablonski diagram. Fate of molecules in electronically excited states. Radiative and nonradiative processes.	2
Lec11	Absorption and emission ultraviolet and visible radiation.	2
Lec12	Basics of nuclear magnetic resonance spectroscopy.	2
Lec13	Nonlinear spectroscopies.	2
Lec14	Review of theoretical methods to simulate molecular spectra.	2
Lec15	Student's presentations regarding selected spectroscopic techniques.	2
Total hours:		30

TEACHING TOOLS USED

N1. Lecture at the blackboard
N2. Multimedia presentation

ACHIEVED SUBJECT LEARNING OUTCOMES

Type of learning outcome	Code of learning outcome	Assessment of learning outcome
Knowledge	P8U_W	exam
Knowledge	P8S_WG	exam
Skills	P8S_UW	exam
Skills	P8S_UO	exam
Social competence	P8S_KO	presentation
Social competence	P8S_KR	presentation

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PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] J. Sadlej, Spektroskopia Molekularna, WNT, Warszawa 2002.
- [2] Z. Kęcki, Podstawy spektroskopii molekularnej, PWN Warszawa 2016.

SECONDARY LITERATURE:

- [1] K. Pigoń, Z. Ruziewicz, Chemia Fizyczna (cz. 2), PWN, Warszawa, 2005.
- [2] D. O. Hayward, Mechanika Kwantowa dla Chemików, PWN, Warszawa, 2007.
- [3] Engel, T., Reid, P., Quantum Chemistry and Spectroscopy, 3rd ed. ed. Pearson, Boston, 2013.
- [4] May, V., Kühn, O., Charge and Energy Transfer Dynamics in Molecular Systems, 3rd ed. Wiley-VCH Verlag GmbH & Co. KGaA, 2011.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

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