GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MOLECULAR SPECTROSCOPY, PG_00066059		
Field of study	Spektroskopia molekularna		
Date of commencement of studies	February 2026	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	Obligatory subject group in the field of study Subject group related to scientific research 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
Semester of study	1	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	exam
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Maciej Śmiechowski	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	30.0	0.0	0.0	45

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	45	5.0	25.0	75

Subject objectives

The aim of the subject is to familiarize students with the theoretical basics of selected areas of molecular spectroscopy and the practical application of spectral analysis and quantum chemical calculations in molecular physical chemistry.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	Student calculates molecular spectra (NMR, IR, UV-VIS, etc.) using quantum chemistry methods, and correctly interprets the obtained results from the point of view of molecular structure of the studied compounds.	[SU4] Ocena umiejętności korzystania z metod i narzędzi [SU1] Ocena realizacji zadania
[K7_U02] prepares detailed documentation of the results of independently conducted experiments and analyzes the obtained results, uses professional vocabulary with understanding and prepares and communicates information	The student prepares an individual report on the performed computational experiment, including the analysis and discussion of the obtained results based on available experimental data.	[SU5] Ocena umiejętności zaprezentowania wyników realizacji zadania [SU4] Ocena umiejętności korzystania z metod i narzędzi [SU2] Ocena umiejętności analizy informacji
[K7_W03] recognizes and describes phenomena in the field of physics, including elements of quantum mechanics, solid state physics and nuclear physics, necessary to predict the course of physical phenomena and to solve technical problems	The student uses knowledge acquired in physics and theoretical and quantum chemistry courses to interpret the processes occurring in a molecule due to the absorption or emission of electromagnetic radiation.	[SW1] Ocena wiedzy faktograficznej
[K7_W02] identifies analytical techniques appropriate for solving specific analytical tasks – also in the production plant	The student has knowledge of the theoretical foundations of selected areas of molecular spectroscopy (IR, NMR, UV/VIS, etc.).	[SW1] Ocena wiedzy faktograficznej

Subject contents

Course content – lecture
The basics of spectroscopy: light as an electromagnetic wave, interaction of light with matter: absorption, emission, scattering, laws of absorption, absorption and emission spectra. Rotational spectroscopy: diatomic molecules (rigid and non-rigid rotor model), polyatomic molecules, measurement techniques and applications. Vibrational spectroscopy: harmonic and anharmonic oscillator, normal modes and characteristic vibrations, rotational structure, isotope effects, selection rules, Raman effect, apparatus for the registration of vibrational spectra, Fourier-transform registration of spectra, spectra of gaseous, liquid and solid samples, applications: qualitative analysis, molecular structure determination, studies of intermolecular interactions. Spectrophotometry: electronic states of molecules (ground and excited states), classification of electronic transitions, selection rules, rovibrational structure, chromophores, emmision spectra: fluorescence, phosphorescence, Jablonski diagram, fotochemical reactions, fotodissociation, measurement of emissional and absorptional electronic spectra, applications: qualitative and quantitative analysis, studies of intermolecular interactions. Nuclear magnetic resonance spectroscopy: the nuclear spin, quantum description of the phenomenon, band structure, chemical shift, shielding, J-coupling, longitudinal and transverse relaxation, measuring apparatus, applications of 1H spectra, applications of other selected nuclei spectra. Electron spin resonance spectroscopy: theoretical basis and quantum description, molecules showing an EPR spectrum, spectra registration techniques, fine and hyperfine structure, applications.

Prerequisites and co-requisites

Mathematics I, Physics I, Physical chemistry, Theoretical chemistry I

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Final exam from lecture contents	50.0%	50.0%
Reports form practical exercises	50.0%	50.0%

Recommended reading

Basic literature	1. Z. Kęcki, Podstawy spektroskopii molekularnej, PWN, Warszawa 1998. 2. J. Sadlej, Spektroskopia molekularna, WNT, Warszawa 2002. 3. W. Kołos, J. Sadlej, Atom i cząsteczka, WNT, Warszawa 2007. 4. H. Haken, H.C. Wolf, Fizyka molekularna z elementami chemii kwantowej, PWN, Warszawa 1998.
Supplementary literature	1. Biofizyka. Wybrane zagadnienia wraz z ćwiczeniami, PWN, Warszawa 2008. 2. Fotochemia i spektroskopia optyczna. Ćwiczenia laboratoryjne, PWN, Warszawa 2009. 3. A. Kaczmarek-Kędziera, M. Ziegler-Borowska, D. Kędziera, Chemia obliczeniowa w laboratorium organicznym, Wyd. Naukowe UMK, Toruń 2014.
eResources addresses	

Example issues/ example questions/ tasks being completed

Bouger-Lambert and Lambert-Beer laws of absorption, the law of additivity of absorption.

Approximate energetic ranges of basic spectroscopic methods.

Einstein's mechanism: forced absorption, stimulated emission, spontaneous emission.

Separation of the electronic Schrödinger equation. Adiabatic and Born-Oppenheimer approximation. Separation of translational, rotational and oscillatory degrees of freedom.

Rigid rotator model. Rigid rotator energy levels, rotation constant, rotation term.

Influence of the oscillatory state of a molecule on rotational spectra.

Basic information about the spectra of polyatomic rotators.

Energy levels of a quantum harmonic oscillator, zero point vibrational energy.

Energy of an anharmonic oscillator, change of selection rules. Mechanical and electrical anharmonicity.

Selection rules in rotational-vibrational spectroscopy.

Stokes and anti-Stokes branch, intensity of Raman bands.

Measurement of the degree of depolarization and its applications.

Methodology of Raman spectroscopy.

Franck-Condon rule, perpendicular and adiabatic electronic transitions.

Chromophores.

Electronic spectra of transition metal ions, high and low spin complexes.

Emission spectra: fluorescence, phosphorescence.

g-factor and the magnetic moment of the nucleus.

Field sweeping and frequency sweeping in NMR measurements.

Magnetization vector, longitudinal and transverse relaxation.

Practical activites within the subject	Not applicable

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