



## Subject card

Subject name and code	MOLECULAR SPECTROSCOPY, PG_00066059						
Field of study	Chemistry						
Date of commencement of studies	February 2025		Academic year of realisation of subject		2024/2025		
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						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Maciej Śmiechowski				
	Teachers		dr hab. inż. Maciej Śmiechowski				
Lesson types and methods of instruction	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_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] Assessment of factual knowledge		
	[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] Assessment of factual knowledge		
	[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.		[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task		
	[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.		[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools		

Subject contents	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, emission spectra: fluorescence, phosphorescence, Jablonski diagram, photochemical reactions, photodissociation, 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 <sup>1</sup> H 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
	Reports form practical exercises	50.0%	50.0%
	Final exam from lecture contents	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	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed	<p>Bouger-Lambert and Lambert-Beer laws of absorption, the law of additivity of absorption.</p> <p>Approximate energetic ranges of basic spectroscopic methods.</p> <p>Einstein's mechanism: forced absorption, stimulated emission, spontaneous emission.</p> <p>Separation of the electronic Schrödinger equation. Adiabatic and Born-Oppenheimer approximation. Separation of translational, rotational and oscillatory degrees of freedom.</p> <p>Rigid rotator model. Rigid rotator energy levels, rotation constant, rotation term.</p> <p>Influence of the oscillatory state of a molecule on rotational spectra.</p> <p>Basic information about the spectra of polyatomic rotators.</p> <p>Energy levels of a quantum harmonic oscillator, zero point vibrational energy.</p> <p>Energy of an anharmonic oscillator, change of selection rules. Mechanical and electrical anharmonicity.</p> <p>Selection rules in rotational-vibrational spectroscopy.</p> <p>Stokes and anti-Stokes branch, intensity of Raman bands.</p> <p>Measurement of the degree of depolarization and its applications.</p> <p>Methodology of Raman spectroscopy.</p> <p>Franck-Condon rule, perpendicular and adiabatic electronic transitions.</p> <p>Chromophores.</p> <p>Electronic spectra of transition metal ions, high and low spin complexes.</p> <p>Emission spectra: fluorescence, phosphorescence.</p> <p><i>g</i>-factor and the magnetic moment of the nucleus.</p> <p>Field sweeping and frequency sweeping in NMR measurements.</p> <p>Magnetization vector, longitudinal and transverse relaxation.</p>		
Work placement	Not applicable		

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