GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	SPECTROSCOPY, PG_00038884		
Field of study	Chemistry		
Date of commencement of studies	February 2024	Academic year of realisation of subject	2023/2024
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	4.0
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 dr hab. inż. Rafał Grubba	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	30.0	0.0	0.0	60

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	60	10.0	30.0	100

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_K01	Student cooperates with other members of the team performing the experiment, divides the tasks among the members of the group, and afterward (using shared experimental results) produces an individual report of the performed experiment.	[SK3] Assessment of ability to organize work [SK1] Assessment of group work skills
K7_W04	Student gains knowledge on the theoretical foundations of selected areas of molecular spectroscopy (IR, NMR, UV/VIS).	[SW1] Assessment of factual knowledge
K7_W05	Student uses his/her knowledge gained on physics and theoretical and quantum chemistry courses to interpret the changes occuring in the molecule due to the absorption or emission of electromagnetic radiation.	[SW1] Assessment of factual knowledge
K7_U04	Student measures experimentally the NMR, IR, and UV-VIS molecular spectra, calculates such molecular spectra 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, 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	Adresy na platformie eNauczanie: Spektroskopia 2024 - Moodle ID: 36890 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=36890

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.

Work placement	Not applicable

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