University of Gdańsk

Subject card

Subject name and code	Advanced chemistry laboratory - physicochemistry, PG_00054411		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2024/2025
Education level	postgraduate studies	Subject group	Obligatory subject group 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 Polish
Semester of study	1	ECTS credits	2.0
Learning profile	academic	Assessment form	
Conducting unit	Katedra Chemii Fizycznej -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Karol Krzymiński	
	Teachers	dr hab. Karol Krzymiński dr inż. Beata Zadykowicz dr Artur Mirocki	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	20.0	0.0	0.0	20

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	20	4.0	26.0	50

Subject objectives

- Theoretical and practical knowledge of selected aspects of emission spectroscopy and HPLC chromatography;
- Acquiring the ability to operate selected equipment for physicochemical tests;
- Familiarization with the theoretical foundations of structural X-ray imaging of single crystals;
- Learning the basics of conducting an experiment in the field of structural X-ray;
- Familiarization with computational methods used to describe chemical systems at the molecular level;
- Familiarization with methods of data processing and interpretation of physicochemical data.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	- The student takes into account the instructions provided during the exercises in the report; - Actively works in a group over time performing activities; - Actively cooperates with English-speaking students; - Critically analyzes physicochemical problems of medium complexity; - Demonstrates understanding of problems related to with the generation of chemical waste and care to minimize its quantity.	[SK1] oral statement/conversation/ discussion [SK5] implementation of a problem task
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	- The student assesses the usefulness of emission techniques in chemical analysis; - Selects chromatographic columns in terms of separation quality, based on designated parameters; - Interprets and translates data obtained using quantum-chemical methods.	[SU1] oral statement/conversation/ discussion
	[CHEMMU2_U01] Plans and implements chemical experiments of medium complexity.	- The student prepares calibration charts and derives analytical parameters, basing on them; - Determines and explains the rate constants of a chemical reaction based on experimental data; - Applies the basic laws of physical chemistry to process quantum-chemical results.	[SU5] implementation of a problem task [SU6] demonstration of practical skills
	[CHEMMU2_W10] Uses knowledge of the principles of operation of the basic scientific and research apparatus used in chemistry.	- The student explains the principle of operation of a plate luminometer, fluorimeter and high-performance liquid chromatography (HPLC) kit; - Interprets and translates computational data regarding the physicochemical properties of systems; - Explains the principle of operation of the Molden and Gaussian programs.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
	[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	- The student provides and explains the basic photochemical laws; - Gives examples of luminizing substances and their applications; - Cites the requirements necessary for the fluorescence (FL) and chemiluminescence (CL) processes to occur. - Presents the principles of work when performing luminometric analyses; - Provides and explains the basic theoretical spectroscopic methods; - Is able to indicate and explain the most important validation parameters of the HPLC system. - Provides and explains basic theoretical quantum-chemical computational methods.	[SW4] test/exam - oral or written [SW1] oral statement/ conversation/discussion
	[CHEMMU2_W03] Demonstrates extended knowledge in the field of modern measuring techniques used in chemical analysis.	- Student podaje znaczenie parametrów uzyskanych w drodze pomiaru emisji promieniowania (FL, CL) z roztworów; - Student zna i podaje znaczenie najważniejszych parametrów charakteryzujących układ chromatograficzny. - Student podaje znaczenie parametrów parametrów uzyskanych w drodze oblicze kwantowo-chemicznych.	[SW1] oral statement/ conversation/discussion [SW3] text preparation/written work [SW5] implementation of a problem task

Course outcome	Subject outcome	Method of verification
[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	- The student selects physical chemistry methods to describe luminescence processes (FL, CL) in terms of their efficiency and kinetics. - The student selects quantum chemistry methods to describe and model chemical processes.	[SW1] oral statement/ conversation/discussion [SW5] implementation of a problem task
[CHEMMU2_U08] Prepares and presents oral presentations in various fields of chemistry in Polish and English, using acquired knowledge and skills as well as basic sources of scientific information.	- The student prepares a report on the exercises in a group; - Cooperates with people who speak English while performing exercises and processing data; - Notices and explains structure-reactivity relationships in the group of tested compounds; - Prepares a substantively correct and complete report on exercises in the group.	[SU2] presentation/project/paper/ report [SU4] test/exam - oral or written

Subject contents

1. Jabłoński's diagram; Lambert-Beer law; radiative and non-radiative processes; Types of absorption bands in the UV-Vis spectrum; Formation of emission spectra; Basic concepts and laws of photochemistry; Physicochemistry of the fluorescence and chemiluminescence process (FL, CL); Examples and applications of FL and CL; The concept of a luminescence marker and indicator; HPLC chromatographic system and its elements and functions, chromatographic parameters and their determination; validation tests of HPLC columns.2. X-ray structural analysis; Diffractometric measurements; Suppression rule; Friedel's law; Single crystal methods (Laue, Weissenberg, rotated crystal, retigram); Determination of crystal structures; Crystallization and single crystals; Crystallographic data processing; Solving and refining the crystal structure.3. Internal and Cartesian coordinates; Ab initio, semi-empirical methods and density functional theory; Geometry optimization, determination of physicochemical properties and characteristics of atoms and chemical molecules; Determination of solvation effects; Thermodynamics of chemical reactions based on quantum chemistry; Prediction of spectral characteristics using quantum mechanics methods.

Prerequisites and co-requisites

Basic requirements:Knowledge of the English language; Basic knowledge of MS Office (Excel, Word) or related programs; Knowledge of the basics of measurement error analysis.Additional requirements:- Knowledge of the basics of X-ray structural analysis: Diffractometric measurements; Suppression rule; Friedel's law; Single crystal methods; Determination of crystal structures; Crystallization and single crystals; Crystallographic data processing; Solving and refining the crystal structure.- Knowledge of the basics of electron spectroscopy: Lambert-Beer law; Jabłoński's diagram; Basic concepts and laws of photochemistry; Applications of UV-Vis absorption and fluorescence; Spectroscopic data processing.- Internal and Cartesian coordinates; Ab initio, semi-empirical methods and density functional theory; Geometry optimization, determination of physicochemical properties and characteristics of atoms and molecules; Determination of solvation effects; Thermodynamics of chemical reactions based on quantum chemistry; Prediction of spectral characteristics using quantum mechanics methods.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Laboratory exercise report	51.0%	50.0%
Theory test	51.0%	50.0%

Recommended reading

Basic literature	1. P.W. Atkins, Physical Chemistry, PWN, Warsaw 2001.2. S. Paszyc, "Basics of photochemistry", Scientific Publishing House PWN, Warsaw, 1992.3. Bojarski, M. Gigla, K. Stróż, M. Surowiec, Crystallography, PWN Scientific Publishing House, 1996.4. Z. Trzaska Durski, H. Trzaska Durska, Basics of structural crystallography and X-ray, PWN, 1994.5. J.B. Foresman, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 1996.6. L. Piela, Ideas of quantum chemistry, PWN, 2011.
Supplementary literature	P. Suppan, Chemistry and light, PWN, Warsaw 1997.W. Zieliński, A. Rajca (eds.), Spectroscopic methods and their application to the identification of organic compounds, PWN, Warsaw, 1995.A. M. Garcia-Campana, W.R. G. Bayenes, "Chemiluminescence in Analytical Chemistry", Marcel Dekker, Inc., New York 2001.Luger, Structural X-ray of single crystals, PWN, 1989.A. F. Wells, Structural inorganic chemistry, WNT, 1993.T. Penkala, Zarys Crystallografia, PWN, 1976. .F. Jensen, Introduction to Computational Chemistry, Wiley, 2007.

	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	Practical part - examples:- Construction of a calibration chart and reading of the component content based on FL emission measurements;- Calculations of the number of theoretical plates and selectivity, based on HPLC chromatograms- Graphical determination of kinetic constants based on recorded reaction time profiles (CL).Theoretical part - examples:- For chemiluminescence to occur, it is necessary...- Selectivity () is a concept that defines...- The emissive processes in Jabłoński's diagram are...	
Work placement	Not applicable	

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