UNIWERSYTET GDAŃSKI

Course title
Advanced chemistry laboratory – Physicochemistry / Laboratorium zaawansowanej chemii – fizykochemia

ECTS code
13.3.0485

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	**Type**	**Form**	
Chemistry	Masters	Full-time studies	

Teaching staff
Ph.D, D.Sc. Karol Krzymiński, Assoc. Prof.; PhD. Eng. Beata Zadykowicz, M.Sc. Artur Mirocki

Forms of classes, the realization and number of hours

Forms of classes, in accordance with the UG Rector's regulations
Laboratory

The realization of activities
classes in the laboratory of physical chemistry;
classes in the computer room

Number of hours
20

ECTS credits

Classes: 20 hours
Consultations: 5 hours
Student's own work: 25 hours
TOTAL: 50 hours - 2 ECTS

The academic cycle
First year, winter semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods

Performing physicochemical experiments; data processing and analysis.
Performing exercises and calculations using a computer.

Form and method of assessment and basic criteria for evaluation or examination requirements

Final evaluation, in accordance with the UG study regulations
Credit for a grade

B. Assessment methods
Test exam, on-time submission of lab report

The basic criteria for evaluation or exam requirements
Team performance of the experimental part covered by the course program; Elaboration of obtained results in the form of detailed laboratory report. The final grade bases on the activity and preparation for laboratory work, quality and punctuality of provided reports and the degree of completion of final theoretical test. In case of failure of the test, completion of theoretical part is required the form of oral answer to questions concerning the contents of course.
To obtain a positive grade, at least 50% of the obtainable points from each stage are required; Failure to complete the

	experimental part, failure to submit a correctly completed report gives no grounds for passing the course.

Required courses and introductory requirements

Completed courses in mathematics, physics, general chemistry and physical chemistry.

English spoken and written; Basic knowledge of MS Office environment (Excel, Word) or related programs; Basic knowledge concerning the analysis of experimental errors.

Aims of course

Practical acquaintance with applications of emission spectroscopy; Principles of fluorescence (FL), chemiluminescence (CL) and electronic absorption (UV-Vis) measurements.

Practical knowledge of methods for assessing the quality of high performance liquid chromatography (HPLC) system; Basics of HPLC column validation.

Expanding theoretical knowledge regarding the emissive processes (FL or CL) and their applications in analysis.

Acquiring the skills to use research equipment for measuring the emission (FL or CL) and UV-Vis absorption spectra and individual recording chromatograms using HPLC systems.

Acquainted with the methods of data processing and interpretation of electronic spectra (CL, FLU, UV-Vis).

Determination of some spectral parameters based on spectra. Elements of fluorescent quantitative analysis.

Familiarization with the theoretical principles of single crystal X-ray crystallography.

Understanding the basics of individual experiment in the field of structural X-ray crystallography.

Understanding the basics of independent experiment in the field of emission spectroscopy or HPLC chromatography.

Introduction to computational methods used to describe chemical systems at the molecular level.

Understanding the basics of individual quantum-chemical calculations. Understanding the basics of independent processing and interpretation of data obtained in quantum-chemical calculations.

Contents

X-ray structural analysis; Diffractometric measurements; Quenching rule; Friedel's law; Methods of monocrystal analysis (Laue’s Weissenberg’s, rotated crystal, retigram); Determination of crystal structures; Crystallization and separation of monocrystals; Processing of crystallographic data; Solving and refining the crystal structure.

Jabłoński's diagram; Lambert-Beer’s law; radiative and non-radiative processes; Types of UV-Vis absorption bands; Principles formation of emission spectra; Basic photochemical laws; Fluorescent (FL) and chemiluminescent (CL) systems; Applications of luminescence; Requirements for the FL and CL process to occur; Experimental parameters describing the CL process; Idea, construction and applications of luminescent labels and indicators.

Parameters of chromatographic (HPLC) separation (coefficients of chromatographic retention, selectivity, resolution, tailing) – definitions and formulas; Construction of the HPLC setup; Validation tests of HPLC columns; Description of HPLC columns; Factors affecting the quality of chromatographic separation.

Internal and Cartesian coordinates; Ab initio, semi-empirical methods and density functional theory (DFT); Optimization of geometry; Determination of physicochemical properties and characteristics of atoms and molecules; Determination of solvation effects; Thermodynamics of processes based on quantum chemistry; Predicting spectral characteristics by quantum mechanics methods.

Bibliography of literature

A. Literature required to pass the course

Electronic materials prepared and provided online by the lectures

B. Extracurricular Reading

P. Atkins, J. de Paula, J. Keeler, “Atkins' Physical Chemistry”, Oxford Press 2017 (11-th or previous editions).
W. Massa, “Crystal Structure Determination”, Springer.
E. Rodriguez, N.G. Swacki, T. Szwacka,. “Basic Elements of Crystallography”, Scribd Publishing.
P. Suppan, „Chemistry and Light”, RSC Publishing, 1994.
A. M. Garcia-Campana, W.R. G. Bayenes, „Chemiluminescence in Analytical Chemistry”, Marcel Dekker, Inc., New York 2001.
J.B. Foresman, “Exploring Chemistry with Electronic Structure Methods”, Gaussian Inc. ,1996.
F. Jensen, Introduction to Computational Chemistry, Wiley, 2007.

Knowledge

Student knows the theoretical basis of X-ray structural analysis; Knows monocrystalline test methods; Knows the practical basics of diffractometric measurements with the participation of the modern research equipment from Oxford Instruments; Knows the principles of crystallographic data processing, solving and refining the crystal structure; Knows what they consist of and what are the conditions for the occurrence of emission processes in organic molecules.

Student knows and understands the energy diagram of the luminezing system; Knows mechanisms of basic chemilunogenic reaction described in the instructions; Knows basic photochemical laws; Knows physicochemical principles of electromagnetic absorption and emission processes;

Student explains the transformations occurring in the electronically excited states of molecules using the Jabłoński’s diagram; Gives examples of substances capable for FL and CL and their applications; Knows the parameters used to characterize emissive processes (quantum yield , integral efficiency; radiation decay constant).

Student knows basic quantum chemical methods for assessing thermodynamic properties of molecules; Knows methods used for predicting electronic absorption and emission spectra.

Skills

Student knows the basics of operation a plate luminometer or stationary spectrofluorimeter or basic HPLC system; Performs qualitative analysis of the electronic spectra of organic compounds; Performs quantitative analysis basing on fluorescence measurements; Runs samples chromatographically and process data; Assesses HPLC column quality using experimental data and formulas; Prepares HPLC mobile phase and exemplary diagnostic mixture.

Student uses the basic equations used in the X-ray structural analysis of single crystals; Interprets results obtained by X-ray structural analysis; Crystallizes chemical compounds subjected do X-ray analysis; Selects single crystals and performs preliminary assessment for their suitability in crystallographic analysis.

Student knows the basics of operation of Molden and Gaussian programs; Interprets results obtained by computational chemistry methods; Uses laws of physical chemistry in processing data obtained by quantum-chemical calculations.

Social competences

Student works in a team: performs measurements, analyzes and develops research results.

Demonstrates responsibility for timely completion of assigned tasks.

Understands the need to deepen his/her knowledge and further education.

Student is able to obtain and develop information from various sources (original scientific literature, monographs, the Internet).

Student understands the need to be familiar with current literature on the subject; Demonstrates creativity in the individual acquisition and processing of scientific information. Demonstrates commitment and creativity to the task and understands its research nature; Knows the role of understanding and theoretical self-preparation while experimenting with high-class research equipment.

Student applies safety procedures during laboratory work.