Course title: Laboratory of advanced chemistry – Physicochemistry

Specialty	Semester	Number of ECTS	Number of hours in the class	Form
Foreign students	**winter**	**2**	**20**	**Lab class**

Name of lecturer: Assoc. Prof. UG Karol Krzymiński, D.Sc. Artur Sikorski, Ph.D. Beata Zadykowicz

Objective of the course (expected learning outcomes and competences to be acquired)

The major aims of this course are to enable students to become acquainted with:

- processes of the luminescence - fluorescence (FLU), chemiluminescence (CL) and electronic absorption (UV-Vis) of organic compounds;
- methods of standardization of chromatographic columns (RP-HPLC);
- the theoretical issues connected with emission processes and modern chromatography (RP-HPLC);
- the theoretical foundations of structural roentgenography of monocrystals,
- presentation of state-of-the-art and current challenges in the development of quantum-chemical methods
- presentation of the available software to be used for computational chemistry

Upon successful completion of this course, a student should be able to:

- use modern apparatus for the measurement of emission (FLU, CL) and absorption (UV-Vis) spectra;
- use basic chromatographic system to assess the quality of RP-HPLC columns using selected test;
- process of data and interpret the spectroscopic spectra (CL, FLU, UV-Vis);
- conduct by himself structural roentgenography experiments;
- plan and interpret the data of computational experiments.

Prerequisites:

- completed courses in general chemistry, inorganic chemistry, analytical chemistry and physical chemistry and quantum chemistry
- basic knowledge of the English language,
- ability to use MS Office (Excel, Word) or the related programs
- basic knowledge of methods of measurement errors analysis

Teaching methods:

- Laboratory experiments

Course contents

- X-ray structural analysis; Diffraction measurements; The extinction rule (the rule of systematic absences); Friedel's Law; Monocrystal methods (Laue's, Weissenberg's, rotated crystal, retigram); Determination of crystal structures; Crystallization and monocrystals; Data processing; Solving and refinement of the crystal structure.
- Jablonski diagram; Lambert-Beer 's law; radial and non-radial energy transfer; Basic photochemical concepts and laws; The formation of the emission spectra (fluorescence (FL) and chemiluminescence (CL)); Fluorescent and chemiluminescent substances; Applications of FL and CL; The photophysical requirements of FL and CL process. The parameters describing CL process; Requirements for luminescent labels.
- Principles of RP-HPLC chromatography, Parameters of chromatographic separations; RP-HPLC chromatographic set-up. Parameters used characterize the quality of chromatographic columns; Assessment of basic chromatographic parameters.
- Introduction to quantum-chemistry methods; Visualization of chemical molecules; Structure and conformational changes of chemical molecules; Utilizing selected computational methods.

Recommended reading:

A. P.W. Atkins, Physical chemistry.
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.

Assessment methods:

- Class deliverables – execution of the indicated experiments and presentation of their results
- Lab reports;
- Oral exam; End-term test

Language of instruction: English

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