Basic Information:
Course Title: **Synthesis and study of photochromic compounds**
Lecturer: Assoc. Prof. Stela Minkovska, PhD
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Total Teaching Hours: 30 hours.

Annotation (up to 150 words)
The aim of the course is to familiarize doctoral students with the design, synthesis and study of the properties of photochromic compounds. Methods for the synthesis of compounds from the group of spiropyrans, spirooxazines and diarylethenes will be studied. Doctoral students will be introduced to the physical methods for the characterization of photochromic compounds - IR, NMR and UV spectroscopy. The influence of substituents, the environment (solution, solid matrix or ionic liquid) on the properties of the compounds and their application as dynamic biosensors in optical recording and information storage, for optical switches, for solar energy storage, in catalysis, and in optical electronics and bioelectronics will be studied.

Course content (brief description by topics or modules)

Topic / Module 1: Basic methods for the synthesis of spiropyrans, spirooxazines and diallylethenes. The design and synthesis of photochromic compounds involves modifying the photochromic molecule with suitable heteroatoms to have precisely defined properties. Development of new methods for isolating new structures, purification of the resulting new compounds using column chromatography, recrystallization, etc.

Topic / Module 2: Methods for proving the structure of photochromic compounds and studying their main photophysical properties - NMR spectroscopy, elemental analysis, mass spectroscopy, UV-VIS spectroscopy, fluorescence spectroscopy, EPR spectroscopy.

• Physicochemical studies of spironaphthoxazines: studying the kinetics of the opening and closing process using the flash photolysis method, studying the optical characteristics of the open and closed forms, studying the thermodynamic characteristics of the photochromic conversion.

• One-dimensional and two-dimensional NMR spectroscopy - to establish the structure of both forms of the photochromic compound and their complexes.

• Mass spectrometry - to determine the stability of the complexes.

• X-ray structural analysis - when obtaining suitable crystals to study the structure of the complexes.

• Quantum chemical calculations.

Topic / Module 3: Study of the influence of substituents and medium (solution, solid matrix or ionic liquid) on the properties of photochromic compounds.

Topic / Module 4: Application of photochromic compounds as dynamic biosensors in optical recording and information storage, for optical switches, for solar energy storage, in catalysis and in optoelectronics and bioelectronics.

Teaching and assessment methods
Full-time and part-time forms of study.

Competencies acquired as a result of training (3–5 points)

1. Acquisition of basic knowledge of the methods of synthesis of photochromic compounds.
2. Acquisition of knowledge of the main physicochemical methods for the characterization of photochromic compounds - NMR spectroscopy, elemental analysis, mass spectroscopy, UV-VIS spectroscopy, fluorescence spectroscopy, EPR spectroscopy
3. Acquisition of knowledge of the influence of substituents and the environment (solution, solid matrix or ionic liquid) on the properties of photochromic compounds.
4. Acquisition of knowledge of the application of photochromic compounds as dynamic biosensors in optical recording and information storage, for optical switches, for solar energy storage, in catalysis, and in optical electronics and bioelectronics.

Literature:

1. Organic photochromic and thermochromic compounds / Ed.: J. C. Crano, R. J. Guglielmetti. New York: Plenum Press, 1999. Vol. 1, Vol. 2
2. Photochromism: molecules and systems / Ed.: H. Dürr, H. Bouas-Laurent. Amsterdam: Elsevier BV, 2003
3. Minkin V. Photo-, thermo-, solvato-, and electrochromic spiroheterocyclic compounds // Chem. Rev. – 2004. – Vol. 104 – P. 2751-2776.
4. Minkovska S.**,** Hadjichristov, G.H, Neacsu, A., Chihaia, V., V. Fedorov, Y. V. Photoswitchable Photochromic Chelating Spironaphthoxazines: Synthesis, Photophysical Properties, Quantum-Chemical Calculations and Complexation Ability. ACS Omega, 9, 4, American Chemical Society, 2024

Additional information (optional) (e.g., special requirements, laboratory equipment, prior knowledge)

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