



ЦЕНТЪР ЗА ОБУЧЕНИЕ – БАИ

1000 София
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Basic Information:

Course Title: Infrared spectroscopy of organic compounds and biomolecules

Lecturer: Denitsa Pantaleeva, Professor PhD, Institute of Organic Chemistry with Centre of Phytochemistry

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Total Teaching Hours: 30 hours

Annotation (up to 150 words)

The course aims to introduce the PhD students and young researchers into the principles of infrared (IR) spectroscopy, the main spectral techniques for spectra measurements in solid state, film and solution as well as their application in the study of organic molecules and biomolecules.

The first part (15 hours) will be focused on the basic theory of vibrational spectroscopy, including a training on the interpretation of IR spectra according to the characteristic vibrational frequencies of various classes of organic compounds. The second part (15 hours) will encompass a practical training for application of the main spectral techniques for IR measurements in the study of organic molecules and biomolecules. Some practical cases of qualitative and quantitative analysis will be introduced such as characterization of structure of synthetic and natural organic compounds, the degree of unsaturation of plant oils, caffeine content in coffee, secondary structure of proteins, lipid structure in solution etc.

Course content (brief description by topics or modules)

Topic 1: Theoretical foundations of Infrared Spectroscopy – Vibrational transitions, characteristic frequencies, and vibrations of a diatomic molecule.

Topic 2: IR Analysis techniques. Factors influencing the position of IR bands – external factors (physical state during measurement), internal (structural) factors, hydrogen bonding, isotope labeling.

Topic 3: Interpretation of IR spectra of saturated hydrocarbons – alkanes; unsaturated hydrocarbons – alkenes, arenes, alkynes.

Topic 4: Interpretation of IR spectra of hydroxyl derivatives – alcohols and phenols.

Topic 5: Interpretation of IR spectra of carbonyl compounds – aldehydes and ketones.

Topic 6: Interpretation of IR spectra of carboxylic acids and their derivatives – esters, anhydrides, acid halides, and carboxylates. Application of IR spectroscopy to the analysis of lipids.

Topic 7: Interpretation of IR spectra of organic compounds containing nitrogen and sulfur – nitriles, nitro compounds, thiols; amines and amides. Application of IR spectroscopy to the analysis of proteins.

Teaching and assessment methods

- 15 academic hours of lectures and 15 academic hours of practical exercises;

- Assessment through the preparation and presentation of a project on topic assigned by the lecturer.



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

- selection and application of appropriate qualitative and quantitative methods for IR analysis of samples varying in type and physical state;
- identification of organic compounds and biomolecules;
- interpretation of the collected data regarding the structure of compounds, their intermolecular and intramolecular interactions, determination of the quantities of individual components in a mixture, and changes resulting from chemical transformations.

Literature:

1. Koji Nakanishi, Infrared Absorption Spectroscopy – Practical, Holden-Day, Inc., San Francisco and Nankodo Company Limited, Tokyo, 1962.
2. Barbara H. Stuart, Infrared Spectroscopy: Fundamentals and Applications, Wiley, 2004, ISBN: 978-0-470-85428-0.
3. S. Bienz, L. Bigler, T. Fox, H. Meier, Spectroscopic Methods in Organic Chemistry, Thieme, 2021.

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

There are no special requirements for the course.