Level: bachelor

Course title: Physical Basis of Modern Methods of Research in Chemistry and Biochemistry

Status: elective

ECTS: 5

Requirements: none

Learning objectives

Introduction to the physical basis of some modern and widely applicable methods of research in chemistry and biochemistry, especially those that are insufficiently or absolutely not studied in the subject of study in higher grades. A wide range of modern physical methods are related to structural analysis of materials at the molecular and supra-molecular level by the methods of scattering of radiation and particles.

Learning outcomes

The ability to recognize the possibilities of penetration into the world of small dimensions at the atomic and molecular level. In particular, X-ray diffraction and other methods of scattering of particles (electrons, neutrons) and radiation.

Syllabus

Theoretical instruction:

Summary of methods of structure analysis based on the study of the spectra of samples (rotational spectrum, infrared and Raman spectra, visible and ultra-violet spectrum, magnetic resonance, mass spectroscopy, etc.) and diffraction images. Scattering of electromagnetic radiation and particles as a method for structural research in chemistry. Fundamentals of crystallography with the study of symmetry of crystal structure. X-ray crystallography – analyzing the crystal and molecular structure by the scattering of x-rays at wide angles (WAXS). Analysis of the material by the small angle x-ray scattering (SAXS). Application of the scattering of neutrons, electrons and light in the analysis of the structure of materials at the micro and macro level. Other physical methods of structure analysis on the supra-molecular dimensional scale: scanning and transmission electron microscopy (SEM, TEM), tunnel microscopy (AFM). Physical basis of non-destructive method for determining the chemical composition: microprobe, X-ray fluorescence analysis (RFA), neutron activation analysis (NNA). Physical basis of the analysis of materials by the thermal methods (modulated DSC, DTG, TM).

Practical instruction:

The choice of crystal samples for X-ray diffraction analysis. Sample mounting techniques and its orientation by the goniometer head. Measurement of the single crystal density by the flotation method and its comparison with the density calculated from the crystal unit cell parameters. Determination of the unit cell parameters and the crystal symmetry on the basis of X-ray diffraction. Determination/calculation of the initial molecular model of the crystal structure and its preparation for refinement. Refinement of the structure model in the isotropic and anisotropic approximation of the thermal oscillations of atoms in the crystal lattice. Determination of the positions of H-atoms in the molecule. Calculating the final parameters of the crystal structure refinement relevant for the publication of results. X-ray diffraction by the crystalline powder, identification of the crystal components in the powder sample.

Weekly teaching load				Other:
Lectures: 2	Exercises: 2	Other forms of teaching:	Student research:	