Infrared spectroscopy, 4.0 credits

Infraröd spektroskopi, 4.0 hp

Third-cycle education course

6FIFMA3

Department of Physics, Chemistry and Biology

Valid from: First half-year 2025

Approved by **Approved**

Registration number

Entry requirements

Entry requirement for studies on third-cycle education courses

- second-cycle degree,
- 240 credits in required courses, including at least 60 second-cycle credits, or
- acquisition of equivalent knowledge in some other manner

Specific entry requirements for this course:
Basic knowledge of modern physics

Specific information

Infrared spectroscopy is a non-destructive tool that provides information about the molecular composition, structure and interactions within a sample, utilizing the fact that molecules vibrate and absorb radiation at specific frequencies in the infrared, and which are characteristic of their structure. Due to its widespread use in many fields of science and engineering, this course is suitable for students in any field interested in chemical or structural sample characterization. The course provides a comprehensive overview of principles, instrumentation and applications in infrared spectroscopy in general, and of Fourier-transform infrared (FTIR) spectroscopy in particular. In addition, selected special applications and methods, as well as other relevant vibrational spectroscopy techniques will also be covered.

Learning outcomes

By the end of the course the students will be able to:

- Understand and explain the theory and the underlying principles of vibrational spectroscopy.
- Understand how FTIR data collection and processing parameters affect the resulting spectra and their resolution.
- Perform IR experiments using different sampling methods
- Process, convert, analyze and interpret IR spectra of different types
- Select a sampling method that is appropriate for a given problem, and to describe typical uses, as well as advantages and limitations of different sampling methods.

Contents

i) Molecular vibrations, light-matter interaction, infrared activity, molecular symmetry, transition dipole moments. Normal modes, overtones and combinations, Fermi resonances.
ii) The Fourier-transform infrared (FTIR) spectrometer and common components in IR optics: sources, detectors, beam splitters, windows, mirrors, polarizers.
ii) FTIR spectroscopy, data collection and processing: Apodization, zero filling, phase errors, spectral resolution. Background spectra, spectral subtraction, baseline correction, quantitative analysis, deconvolution.
iv) Interpretation of spectra: characteristic vibrations, group frequencies, the fingerprint region. Spectra-structure correlations. Examples of compounds in the gas, liquid, and solid phases.
v) Sampling techniques: Transmission, Reflectance (ATR, IRAS, DRIFT), Microscopy, 2D IR, PM-IRAS, vibrational CD, Step-scan FTIR.
vi) Other vibrational spectroscopy techniques: Sum-Frequency Generation (SFG), Inelastic neutron scattering (INS), Raman scattering, Surface-enhanced Raman scattering (SERS), Photoacoustic IR spectroscopy, (EELS), Inelastic electron tunneling spectroscopy (IETS).

Educational methods

The course is organized in lectures, computer exercises, lab classes for experimental work (participants are encouraged to bring their own samples for examination during the laborations), and seminars where the experimental work is summarized and presented.

Examination

Homework exercises distributed after some of the lectures. A written report and an oral presentation summarizing the mandatory experimental work.

Grading

Two-grade scale

General information

The course is planned and carried out according to what is stated in this syllabus. Course evaluation, analysis and suggestions for improvement should be fed back to the Research and PhD studies Committee (FUN) by the course coordinator.