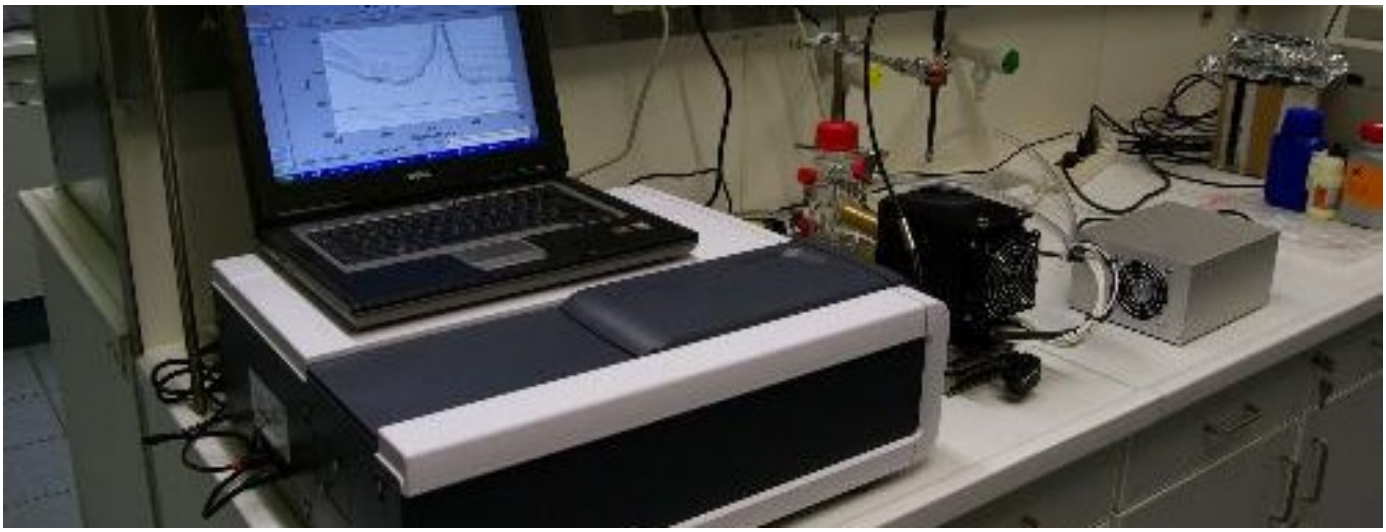
TECHNICAL
EDUCATION
ACADEMY

School of Engineering

COURSE PROGRAMME

000574

PROD017 - Physico-Chemical Analysis Methods: Infrared Spectroscopy Techniques



Learn from the Best in the Business!

Course overview

Intermediate level

Why take this course

The aim of this programme is to develop new competencies and enhance existing ones among chemical industry employees necessary for solving production and technological challenges in quality control and analytical monitoring of technological processes through testing using near and mid-infrared spectroscopy for liquid, bulk, and solid products. It also aims to improve the professional level of employees within their current qualifications.

Participants will be introduced to new types of laboratory instrumental chemical analysis. Key principles of measurement conditions selection will be covered: requirements for reagents and consumables used; main components of analytical equipment; approaches in sample preparation.

This course will enable participants not only to enhance their qualifications and acquire new competencies in IR spectroscopy but also significantly improve the quality and accuracy of analytical control in chemical industry enterprises

Who it is for and how it helps

• Specialists working in laboratories of oil and gas companies engaged in the analysis of raw materials, intermediates, and finished products.

• Laboratory technicians responsible for preparing and conducting spectroscopic measurements.

• Engineers responsible for product quality control and compliance with standards and regulations.

• Specialists involved in developing and implementing quality control methods.

• Professionals responsible for controlling technological processes at oil refining and petrochemical plants.

• Engineers focused on optimizing production processes and ensuring their stability.

• Specialists ensuring the accuracy and reliability of measuring instruments.

• Metrologists responsible for calibration and tuning of analytical equipment.

• Managers overseeing product quality management and analytical laboratory operations.

• Managers coordinating the work of quality and analytical specialists

What you will learn

- Understand the basic theoretical foundations of IR spectroscopy
- Operate IR spectroscopy instruments
- Prepare and record spectra of samples
- Perform qualitative and quantitative analysis
- Develop calibration models

Curriculum

Modules 01–02

01 Theoretical Foundations of IR Spectroscopy

- Physical basics of IR spectroscopy: interaction of matter with IR radiation. The electromagnetic spectrum. IR radiation ranges: near-IR, mid-wave, fundamental ("fingerprint region"), and far (characteristic frequencies)
- Classical theory of molecular vibrational spectra. Quantum mechanical representation of vibrational spectra. Normal vibrations, types of normal vibrations
- Harmonic and anharmonic oscillator models. The nature of overtones and combination frequencies. Energy of vibrational, rotational, and electronic transitions
- Symmetry of molecules. Types of vibrations in polyatomic molecules: stretching, bending (scissor, pendulum, fan, planar, torsional)
- Intensity of vibrations and the selection rule in IR spectra. Factors affecting vibration frequencies
- Main IR spectrum regions of organic compounds. Characteristic frequencies of stretching vibrations of functional groups. Structural-group analysis

02 Instruments and Hardware Setup of IR Spectroscopy

- Structure of instruments and hardware setup for the method. Phenomenon of radiation dispersion. Optical scheme of instruments. Applications and capabilities of IR spectroscopy
- Beer-Lambert-Bouguer law. Sensitivity and contrast of measurement, resolution, and noise
- Single-beam and dual-beam IR spectrophotometers. Instruments with sequential scanning and spectrum recording
- Continuous IR radiation sources: silite rods, Nernst glower from zirconia oxides, globars from rare-earth metal oxides, laser photodiodes, silica-coated incandescent filaments. Radiation ranges, characteristics
- Monochromators in dispersing devices, optical prisms, diffraction gratings, Littrow mirror
- Optical filters in IR spectroscopy: absorbing (quartz, alkali and alkaline earth metal halides), reflecting (ionic crystals), scattering (aluminium plates with rough surfaces, Michelson interferometers)
- IR radiation detectors: bolometers, thermocouples, thermopiles, semiconductor detectors (DTGS, MST, RTS5, LTaO3), photodiodes, diode arrays, avalanche photodiodes, pyroelectric detectors
- Materials for IR devices and cuvettes: helium-neon laser for internal standard, polystyrene films (25–50 μm) for calibration diaphragms, polypropylene films for liquid cuvettes, glass: AMTIR, KRS5, indium and gallium antimonides. Solvents: perchlorocarbon, dichloroethane, carbon disulfide, mineral oil (nujol), perfluorinated oil, standards

Curriculum

Modules 02–03 · Module 02 — continued

- Dual-beam IR spectrometers with Spekord 76 IR type optical zero. Structure and operation. Advantages and disadvantages
- Fourier-transform IR spectrophotometry. Fourier transformation. Michelson interferometer. Fourier spectrometer Varian 660-IR (Agilent Technologies) with TGA/IR attachments, Raman accessory (KR), external module, matrix detection systems, SEM-NRR AS. Structure and operation. Advantages and disadvantages
- Block diagram of a Raman spectrometer with laser excitation of the spectrum. Structure and operation. Advantages and applications of KR spectroscopy of scattering. Advantages and disadvantages

03 Techniques for Recording Spectra of Liquid and Solid Samples: Recording and Processing Spectra

- Methods for sample preparation and measurement techniques for IR spectra of solutions and powders using salt and polymer matrices and liquid cuvettes. Recording and processing of spectra include baseline correction, smoothing, marking, and spectrum calculation (measuring peak height and area)
- Techniques for recording spectra using vacuumed tablets of the substance mixed with KBr powder. Sample preparation with mineral oil for thin-layer technique. Preparation of suspensions for analysis in a liquid cuvette. Analysis of liquid films on the surface of salt windows
- Techniques for recording IR spectra using attachments: diffuse reflection, specular reflection, glancing angle attachment, recording on FTIR spectrometers
- Methods for transmitting IR radiation using multi-path gas cuvettes
- Measurement of spectra of adsorbed molecules using high vacuum sealed flow cuvettes at high temperatures (500-1000°C)
- Techniques for recording with total internal reflection disruption (TIR) in a liquid film or on a crystal surface (TI halides or Zn selenide)
- Techniques for recording diffuse reflection (DRIFTS) on the surface of liquid films or measured powder
- IR analysis method with preliminary separation of sample components by thin-layer chromatography
- Resolution of a Fourier-transform spectrometer, apodization and its impact on spectral characteristics. Ways to improve the recorded spectrum of a Fourier-transform spectrometer

Curriculum

Modules 03–06 · Module 03 — continued

- Techniques for spectrum recording: transmission, single and multiple disrupted total wave reflection (TIR). Accessories, TIR crystals. Choosing analysis techniques depending on the sample's state. Device structure and operation. Advantages and disadvantages

04 Qualitative and Quantitative Analysis in Spectrometry

- Qualitative analysis in near and mid-range IR spectroscopy. Signal characteristics: position, width, amplitude. Patterns of vibration manifestation. Library search (algorithms, creation, and editing of the spectral library). Decoding spectra by frequencies and analytical ranges 3600-3100; 3100-2800; 2800-1800; 1800-1400 cm-1. Baseline method, integral method of spectrogram calculation. Characteristic signals of different classes of organic compounds
- Quantitative analysis in near and mid-range IR spectroscopy, based on fundamental laws of light absorption. Software processing of spectra for quantitative analysis: basic and additional manipulations, conduct algorithm. Processing of IR spectra for quantitative analysis and its algorithm. Multicomponent quantitative analysis
- Overview of standardized measurement methodologies (SMIs) and standards based on the use of IR spectrometry. Application of IR spectrometry in analytical control of oil refining, petrochemical, food, and pharmaceutical industry products

05 Theoretical Foundations of Calibration Model Construction in IR Spectroscopy

- Analysis of variance: fundamental principles. Correlation analysis: tasks, types of relationships, conditions of application, limitations. Covariance and correlation coefficients
- Regression analysis: essence, definition, and tasks. Simple linear regression and least squares method. Approximation error, assessment of statistical significance of the regression model

06 Development of Calibration Models

- Introduction to Principal Component Analysis (PCA) for spectral data analysis
- Introduction to Partial Least Squares (PLS) for spectral data analysis
- Practical issues and features of calibration model development. Use of the Shewhart method

Participation and contacts

Joining the programme

Contact the Academy and quote course code 000574 to confirm dates, delivery format, prices and enrolment terms.

Training for your team

Tell us your business goals, the roles and number of participants, and your preferred dates and location. This will help us discuss the right training option.

Preparing for the programme

The published programme does not specify any prerequisites. Contact us before enrolling to confirm how to prepare.

Discuss your training needs

mail@tecedu.org
www.tecedu.academy

Learn from the Best in the Business!