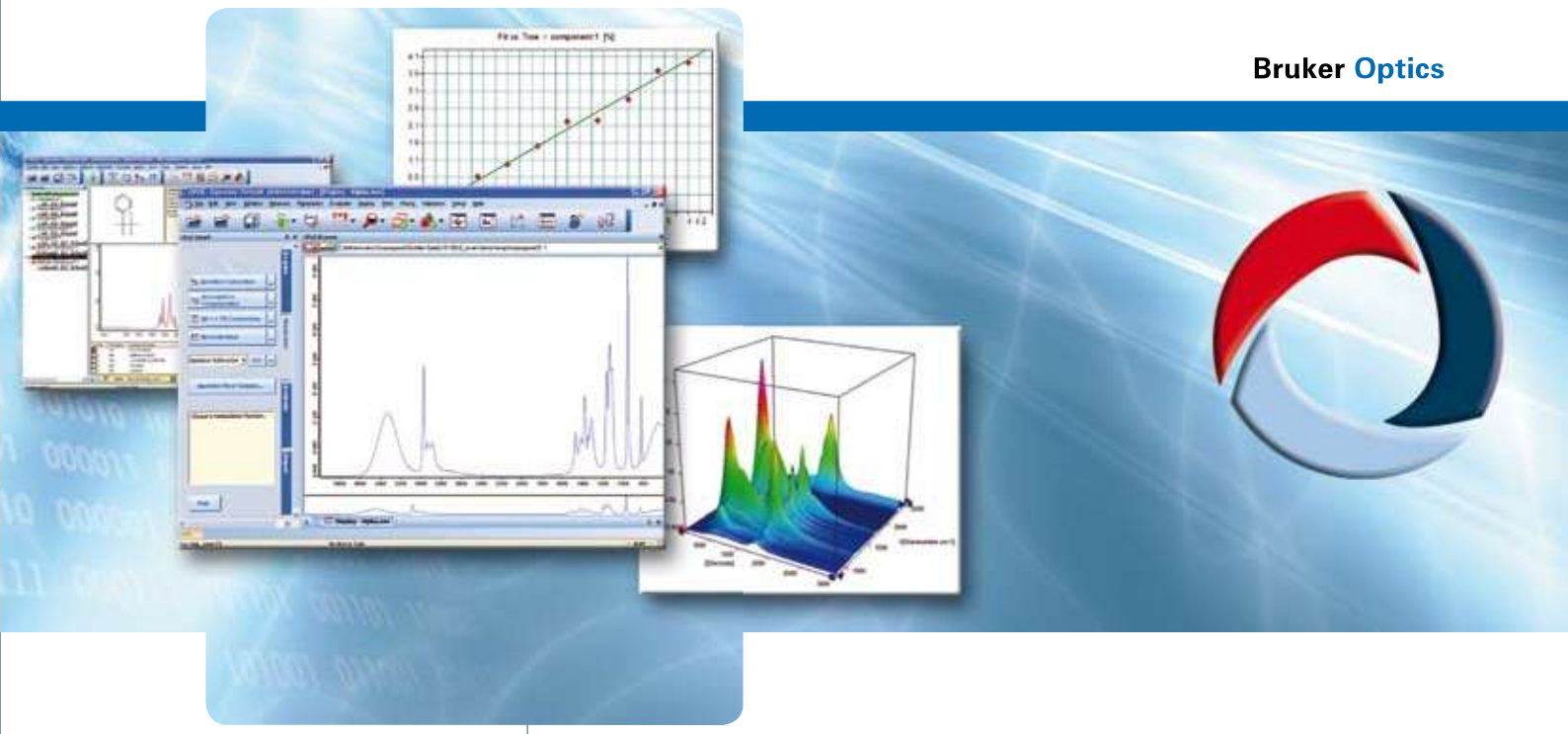
Bruker Optics



OPUS

- Validated Spectroscopy Software
  for Bruker FT-IR, NIR, and Raman Spectrometers

think forward

Software

OPUS Software

OPUS is an easy-to-use, powerful, all-in-one spectroscopy software. It includes the most comprehensive collection of data acquisition, processing, and evaluation functions optimized for applications in the fields of routine laboratory analysis, advanced R&D applications, and process monitoring.

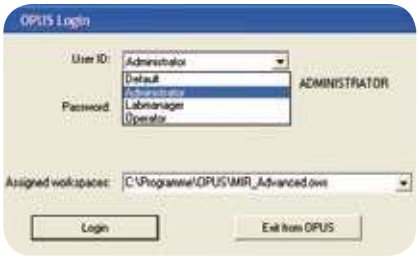
OPUS Software for Infrared and Raman Spectroscopy

- ☑ OPUS is made for you. Easily configure OPUS to your individual needs.
- ☑ Your needs may change, but your software will remain as easy to use as reliable. With available Advanced Software Packages, which are integrated seamlessly into the main program, OPUS adapts itself to fulfill your needs.
- ☑ OPUS has the security you need, and it is GMP compliant.
- ☑ OPUS communicates with you. Several interactive dialogs enable you to take appropriate action to data manipulations and evaluations.
- ☑ OPUS does more than just measuring spectra. The advanced software also monitors the spectrometer continuously, indicating the instrument status in real time to the user.
- ☑ OPUS supports you. Complete on-line multimedia tutorial and maintenance instructions provide you support when its needed.
- ☑ OPUS teaches you. A multimedia tutorial and integrated method-development wizards teach you about infrared theory and data evaluation.
- ☑ OPUS saves you time. By including a range of features from a basic sequence editor to Visual Basic programming tools, OPUS makes it easy to automate your standard procedures.
- ☑ OPUS offers the most comprehensive collection of data processing and evaluation methods available on the market.

Powerful Functions with Individual Interfaces

User Management

OPUS has extended user settings and user management features. User access to OPUS is completely customizable. Maybe your quality control laboratory requires restricted access to the analyzer software. Or maybe you want to benefit from the flexibility and power of OPUS by granting full access for your demanding R&D applications. Either way, OPUS will work with you. OPUS meets all requirements due to its extended user management and user settings.



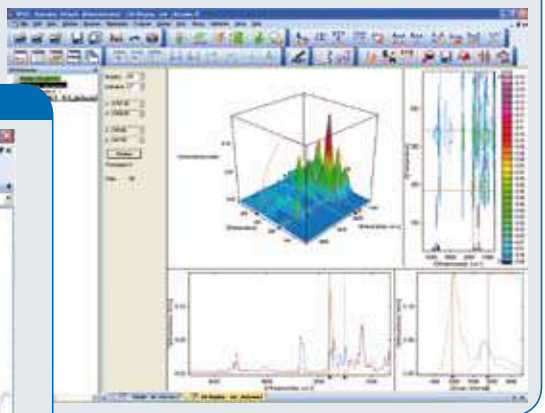
- Individual log in with user ID and password
- Three user levels
- Individual access configuration for each user
- Complete user management functionality
- Unlimited number of users

User Interface

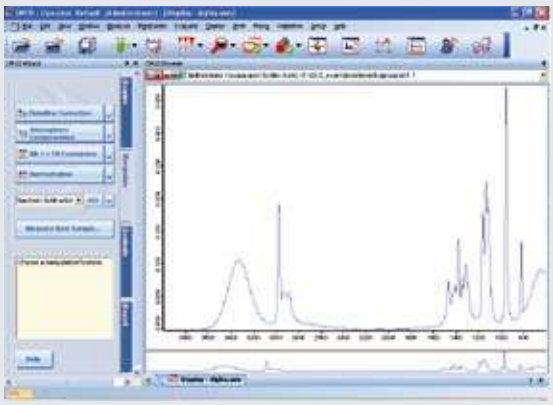
Each user and each field of application has different requirements. In order to meet individual needs, spectroscopy softwares typically come in different "dedicated" stand-alone versions. OPUS philosophy, however, is different. The core of the system is a set of pre-configured user interfaces. Many can be used as is, but they are also easy to customize to fit your needs. That's the power of OPUS's flexibility: as your needs change, the software changes to meet those needs.

- Pre-defined, instrument-specific user interfaces for routine and R&D applications
- Customizable user interfaces for individual requirements: menus, icons, parameters
- Drag & drop functionality
- Interactive dialogs
- OPUS browser for multiple spectra operation
- Multiple window mode
- Extended spectra and result display functionality
- Full multiple file operation capability

OPUS 3D/for kinetic studies



OPUS/Mentor for routine analysis



Secure and Dependable

Data Security

OPUS ensures the safety and integrity of your data.

- No loss of data or overwriting of raw data
- Fully GMP/GLP compatible, prepared for 21 CFR Part 11 conformity
- Automatically generated data history (audit trail)
- All relevant data (measurement parameters, manipulations, evaluation results, reports, images, etc.) are stored in one data file

Spectrometer Diagnostic

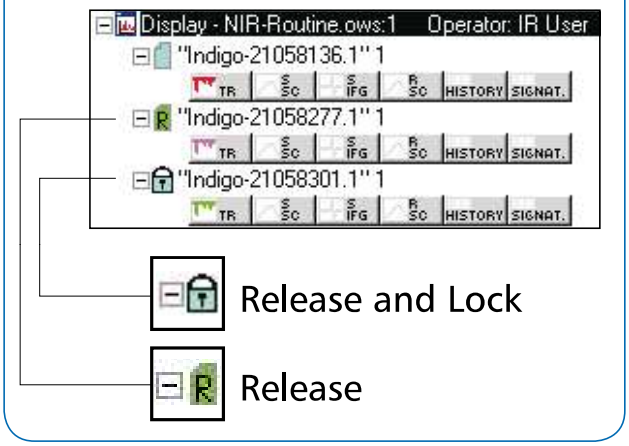
Only a permanently monitored spectrometer can ensure the acquisition of reliable data.
OPUS includes:

- Permanent online diagnostics
- "Real-time" display of instrument status
- Instrument status report
- Integrated automatic instrument tests (OQ, PQ)

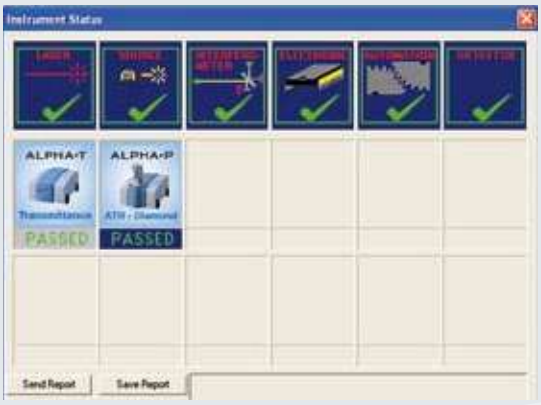
Validation

Today's regulated laboratory and process environments must comply with extensive regulatory requirements. Providing multiple user support, electronic signature records, high level of security and many other required features, OPUS is a fully validated software and the answer to 21 CFR Part 11 requirements.

Electronic Signatures



Spectrometer diagnostic



Bruker offers comprehensive instrument and software validation manuals for this compliance.

Count on Your Results

OPUS provides you the complete set of functions required to convert your spectra into analytical results. Wizards and the complete online help support the user in setting up methods. By design, unlimited numbers of spectra can be evaluated simultaneously with a single mouse click.

Characterize Your Sample

Band Location

The choise is yours:

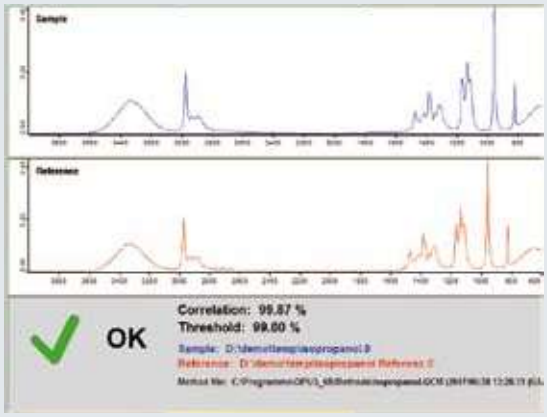
- Automatic, one-click peak picking
- Interactive peak picking: a real-time display shows the results depending on the selected parameters
- Various peak pick algorithms
- Simultaneous evaluation of multiple spectra

The peak pick results are stored in the same file as the spectrum. So you never will search your data.

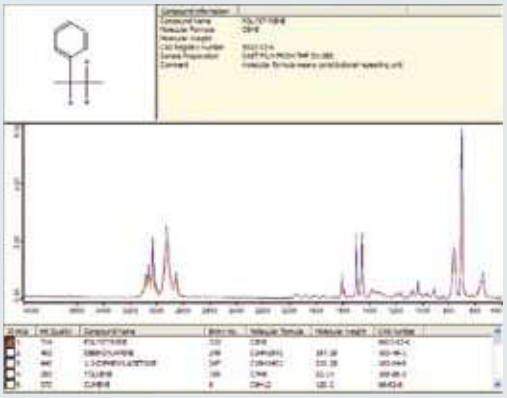
Band Correlation Chart

Find out the chemical structure of your compound using the power of infrared spectroscopy. OPUS easily displays the measured spectrum with a band correlation chart, which shows typical absorption frequencies of various chemical groups.

Compare spectra



Library search



Identify Your Sample

Spectra Comparison with "QuickCompare"

Is the quality of your sample as specified? Use OPUS QC function for your daily MidIR quality control.

- Quick response (OK / NOT OK), correlation related identification, comparison with one spectrum or an average spectrum of a directory
- Comparison with different spectra in a directory without the need to create a spectrum library
- Simultaneous comparison of multiple spectra

Search Spectra in Libraries

What is your sample made of?
Use OPUS's powerful search algorithm to find all necessary information about your sample in commercial libraries. Search simultaneously in different spectrum libraries.

The optional, extended OPUS/SEARCH package contains additional professional search tools.

- Multiple advanced search algorithms
- Information search
- Structure search
- Complete library management

Quantify your sample

Integration

Integrate single bands or multiple regions within your spectrum to get quantitative information. Define the integration parameters once and all of your future integrations can be performed on the basis of those parameters.

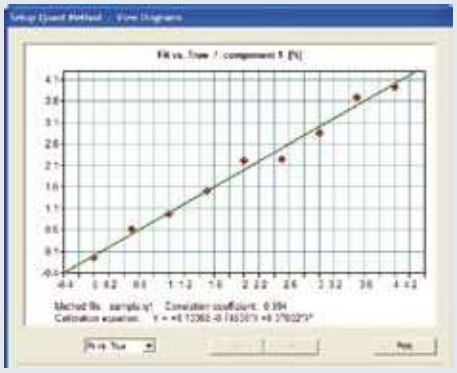
- Interactive setup
- Integrated areas are shown together with the spectrum in the display
- 18 different integration modes are available including integration of several peaks in a spectrum
- Simultaneous integration of multiple spectra

Quantification

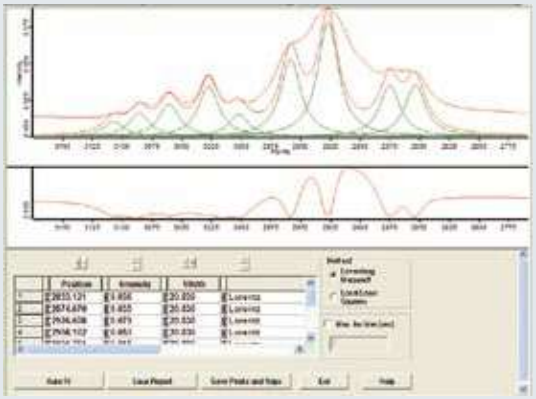
According to Lambert Beer's law, infrared absorption is proportional to the concentration of the analyzed molecules. Easily build up your individual quantification method (according to Lambert-Beer) in order to analyze your samples.

- Wizard for easy method setup
- Various integration modes (integration of peaks area or peak heights)
- Different calibration models (linear and polynomial)
- Calibration results are displayed as table and curve
- The quantification results are stored in the same file as the spectrum
- Simultaneous quantification of multiple spectra

Quantitative analysis



Curve fit



Study Your Sample

Curve Fit

Curve fit is finding the individual line segments which best fit to a measured spectrum by calculating their individual absorbance, line shape and intensity.

- Set up individual frequencies by mouse
- Selection of Levenberg-Marquard algorithms or Local Least Square calculation
- Interactive manipulations
- Lorentzian, Gaussian or mixed curve shape selection
- Interactive residuum calculation
- Interactive solution display

Self Deconvolution

Self Deconvolution is a routine function for resolving intrinsically overlapped bands. The aim of deconvolution is to decrease the width of all lines in a limited spectral region.

- Interactive or numerical selection of bandwidth
- Interactive or numerical noise reduction
- Gaussian or Lorentzian function
- Frequency range selection

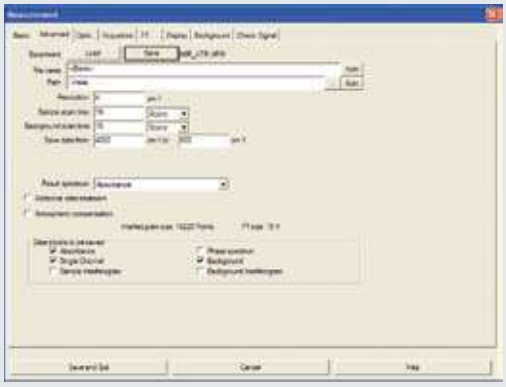
Measure, Process, and Present

Measurement Manager

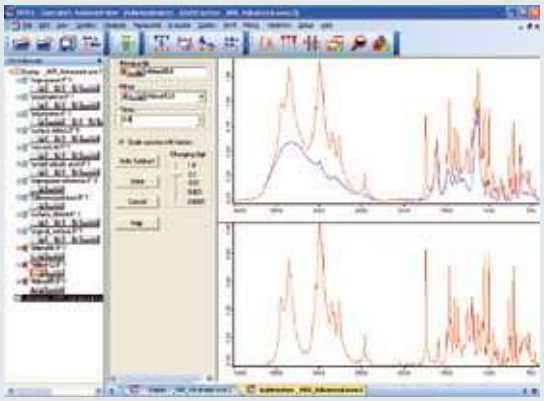
You can start your measurement with a single mouse click or customize the measurement parameters to your individual needs and save them as an individual parameter set.

- Pre-defined parameter sets for all common applications
- Pre-scan real-time display to check the spectral quality before measurement
- Observe the spectra during measurement
- Single and repeated measurements
- Measurement can be embedded in defined sequences
- You never lose any data. Measurement results are saved automatically including the complete parameter set.
- Multitasking: perform data processing or evaluation while measurements are running

Expert measurement setup



Interactive data processing



Data Processing

OPUS provides a large number of spectrum manipulation functions from basic data processing such as base line correction up to high end manipulations which are indispensable for demanding research applications.

- Interactive functions for easy parameter selection
- Simultaneous treatment of an unlimited number of spectra
- All data processing functions can be operated with 3D files (from chromatographic, mapping or imaging results)

Most common manipulation function in OPUS:

- Atmospheric compensation
- Complete set of pre-treatments needed for data evaluation
- Spectrum subtraction (automatic and interactive)
- Several spectrum conversions
- Averaging
- Spectrum calculator
- Complete set of post-run FT processing

OPUS supports you by documenting your analytical work even if you print or present your results in other programs.

Print

- QuickPrint, WYSIWYG with one mouse click
- OPUS offers various predefined print layouts. Use the powerful layout-editor to customize the layout to your individual needs
- Print all results together: spectra, parameters and evaluation results

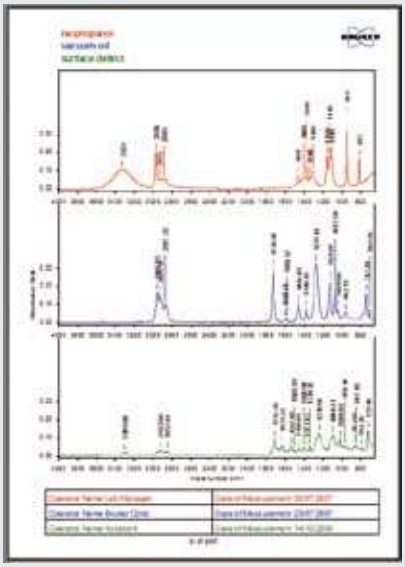
Present

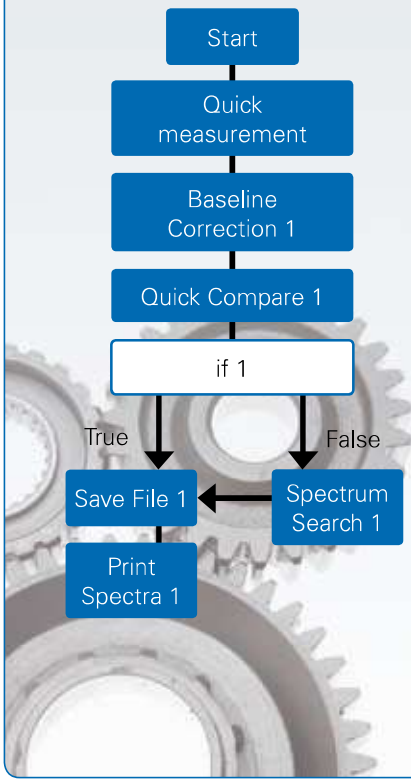
Share your results with colleagues worldwide.
Easily copy & paste your spectra to external presentation programs.

Journalize

Summarize your personal work with OPUS lab journal. This tool lists your results by time or category, whichever you prefer.

OPUS Reports





Automate Your Procedures

For repetitive/recurring sequences, OPUS provides various possibilities for automation. The graphical sequence editor offers inexperienced user an easy way to create individual automated sequences. Experienced operators have the ability to automate advanced sequences, data processing and external communication connections with macros and Visual Basic scripts.

Graphical Sequence Editor:

- Measure, process, evaluate, and report with only one mouse click
- A Wizard guides the user step by step through the creation procedure.
- Integrated error management
- Add your sequence to OPUS menus and icons
- No programming skills are required
- Pre-defined FT-IR spectroscopy sequences
- Sample preparation techniques and measurement modes.
- Data evaluation
- Spectra interpretation

Libraries

Before digital data processing became prevalent, spectra were recorded on paper and compared with analyzed data by hand. Nowadays, digital spectrum collections (libraries) offer a faster, more effective way to compare analysis results. Infrared libraries have been used since the beginning of this digital revolution.

Many infrared libraries are available now, that are categorized by chemical classes, constitution, aggregation state, and even intended use (i.e. environmental protection, homeland defense, etc.)

BRUKER databases are designed for use in:

- Polymers
- Polymer additives
- Fillers
- Inorganic compounds
- Natural fibers
- Synthetic fibers
- Laboratory chemicals
- Vapor-phase compounds
- Drugs
- Kidney stones

Access the largest collection of infrared spectra!

The worldwide digital IR-spectrum collection meanwhile consists of more than 500,000 spectra.
In addition to the spectrum and chemical name, digital databases contain a lot more information on the chemical compound identified, such as structure, CAS identification number, boiling and melting point, and toxicity.

Revolutionary search algorithm - having an eye for the esssential

In contrast to the classical approach, Bruker Optics' new algorithm takes the main characteristic of an IR spectrum; the presence of various sharp peaks, into account when comparing a measured infrared spectrum with a database. A unique three level database search compares the peak position, relative intensities and the peak half width. No data pre-treatment has to be used, which makes the algorithm very simple to use. This procedure weights the areas in the spectrum where peaks are present stronger than regions without peaks. This unique algorithm allows to find ATR spectra in transmission libraries and identify components in mixtures.

- Rapid and reliable identification
- Find ATR spectra in transmission databases
- Identify components of mixtures

Support

OPUS provides answers to many questions from the basics of IR spectroscopy presented in an OPUS tutorial, to practical information about the OPUS functions and instrument maintenance.

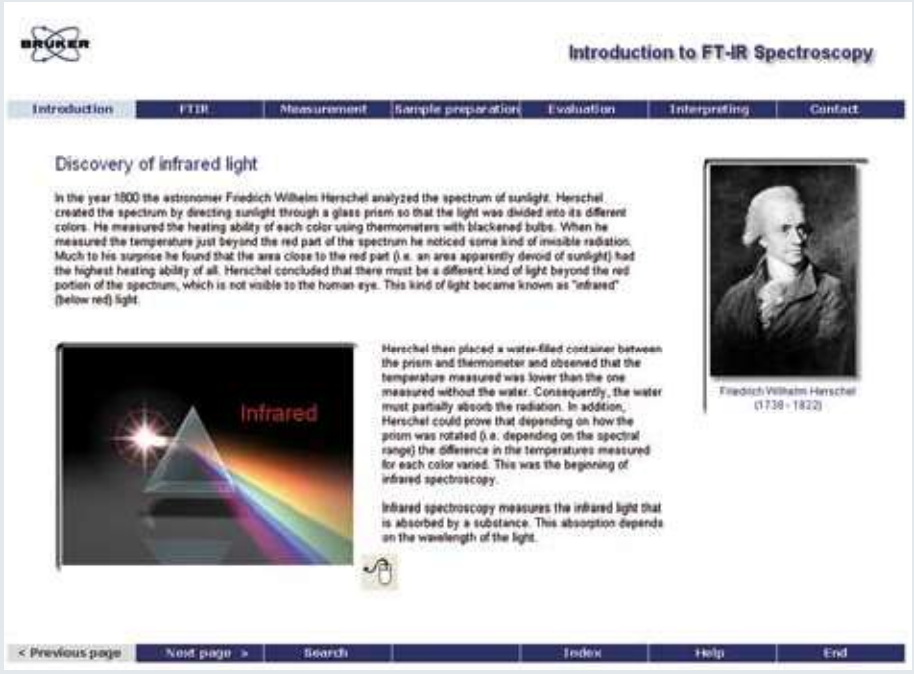
FT-IR Tutorial

- Theory of infrared spectroscopy
- Sample preparation techniques
- Measurement techniques
- Data evaluation
- Spectra interpretation

OPUS Online Help

- Permanently available when working with OPUS
- Access to full OPUS user manuals

FT-IR tutorial



• OPUS Software Packages

The OPUS standard package is an easy-to use and powerful spectroscopy software, which covers all the demands of routine analysis. The outstanding flexibility of OPUS is based on the variety of optional software packages for the individual needs of each analytical laboratory. OPUS packages, which cover all specialized spectroscopic applications, are integrated seamlessly into the main program.

LAB	▪ Easy user interface for quality control by identification or quantification of lab samples.
IDENT	▪ Setup, validation and use of hierarchical identification libraries, including statistics for individual materials.
QUANT	▪ Multivariate quantification based on PLS (Partial Least Squares) calibrations, including optimization tools.
VALIDATION	▪ Allows to work in a validated environment, according to the FDA regulation 21 CFR Part 11
SEARCH	▪ Advanced library search and administration
STRUCTURE	▪ Drawing of chemical structures and their integration into the user spectrum library
MAP	▪ Automatic data acquisition using computer-controlled XY-sample stages
VIDEO	▪ Video-assisted measurement and interactive data evaluation
3D	▪ Viewing, processing and plotting of 3D files resulting from mapping, imaging or kinetic measurements
CHROM	▪ Acquiring and processing data/spectra resulting from coupled techniques, e. g. TG-IR
SEMI	▪ Intended for quality control of semiconductors
STEP	▪ Intended for measurements in step-scan mode
PROCESS	▪ Cyclic data aquisition with trend display, including communication with the process control system.

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