INVENIO S

User Manual

1861146

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This manual is the original documentation for the FTIR spectrometer INVENIO S. The description given in this manual is based on the technical specifications and the technical design valid at the time of publication. Technical specifications and technical design may be subject to change.

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1 Safety

1.1 General safety information

- Read carefully all instructions and safety notes in this manual before installing and putting the spectrometer into operation. Keep this manual for future reference available at any time.
- Always observe the instructions and safety notes given in this manual. Failure to do so can lead to personal injuries and/or property damage. Non-observance of the instructions and safety notes will violate the intended use of the spectrometer. (See section 1.5.)
- It is the operator's duty to plan and implement all necessary safety measures and to supervise their observance. Moreover, the operator must ensure that the spectrometer is in proper condition and fully functioning.
- A safe and trouble-free operation of the spectrometer is ensured only if all components of the analysis system are installed, operated, maintained and repaired according to the procedures described in this manual and in compliance with all relevant safety standards and regulations.
- The spectrometer should be operated only by authorized personnel who are trained in operating the spectrometer and who are familiar with the relevant safety instructions.
- Never remove or deactivate any supporting safety systems during spectrometer operation. Objects and/or material not required for the operation should be kept outside the operating area of the spectrometer.

The spectrometer complies with the IEC/EN 61010-1 safety regulations.

1.2 Classification of the safety notes

Depending on the degree of hazard, important safety notes are classified in this manual by signal words as follows:

⚠ WARNING

- Indicates a hazardous situation which, if not avoided, could result in death or serious injury.

⚠ CAUTION

- Indicates a hazardous situation which, if not avoided, could result in minor or moderate injury.

NOTE

- Indicates a hazardous situation which could result in material damage if the appropriate safety instructions are not observed.

i The symbol i will draw your attention to additional pieces of information which might be useful for you.

1.3 Overview of possible types of hazard

1.3.1 Possible hazards during installation, operation and maintenance

Hazards that can possibly occur during installing, operating and repairing the spectrometer are indicated by the appropriate warning labels on the spectrometer. The following warning labels indicate different dangerous situations which may be caused by an improper use of the analysis system:

Warning symbol	Definition
	**General hazard:** This warning symbol indicates a general hazard. The label is located near the danger spot in question. Observe the safety instructions and follow the precautions described to avoid personal injury and/or property damage.
	**Laser radiation:** This warning symbol indicates the existence of laser radiation. The label is located near the aperture at which hazardous laser radiation exits the instrument. Do not look directly into the laser beam or use any kind of optical instruments to look into the beam as this may cause permanent eye damage.
	**Electrical shock:** This warning symbol indicates an electrical hazard. The label is located near live parts or on housings behind which are live parts that represent an accidental contact hazard. Do not touch these parts. Before removing the corresponding housing and beginning any maintenance or repair work, first turn off the main power switch and unplug the main power cable. Ensure that all live parts do not come into contact with a conductive substance or liquid. Non-observance of these safety instructions can cause severe personal injury and/or property damage.
	**Danger of frostbite:** This warning symbol indicates cryogenic liquids (e.g. liquid nitrogen) required to operate the spectrometer (e.g. cooling the detector). Exposure to these liquids or cooled components causes frostbite effects. Handle the liquids with utmost care. Observe the safety instructions for operating with cryogenic liquids. Potential hazards: Cooling a MCT detector with liquid nitrogen
	**Hot surface:** This warning symbol refers to components and surfaces which can become very hot during the spectrometer operation. Do not touch these components and surfaces. Risk of skin burn! Be careful when operating near hot components and/or surfaces. Potential hazards: heatable measurement accessories (e.g. heatable ATR unit)
	**Toxic material:** This warning symbol indicates a toxic material. Skin and/or eye contact, inhaling and/or swallowing a toxic material cause serious health problems. Consult the safety data sheet and observe the safety instructions for the toxic material in question. Potential hazards: toxic window material (e.g. ZnSe)

Warning symbol	Definition
	**Harmful material:** This warning symbol indicates a harmful material. Skin and/or eye contact, inhaling and/or swallowing a harmful material can cause health problems. Consult the safety data sheet and observe the safety instructions for the harmful material in question. Potential hazards: harmful window material (e.g. CsI)

Important: All warning labels on the spectrometer must always be kept legible. Immediately replace a worn or damaged label!

1.3.2 Possible hazardous sample materials

There can also be hazards caused by the sample material. Depending on the type of hazardous substances you work with, you have to observe specific substance-relevant safety instructions. Affix the corresponding warning label at the appropriate place at the spectrometer. The label must be well legible and permanently discernible. The following list contains some examples of hazardous substances:

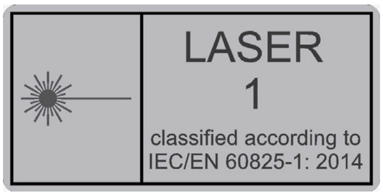
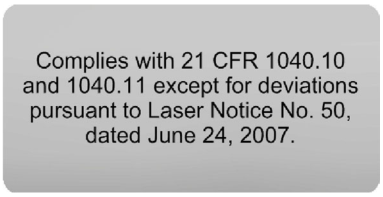
Symbol	Definition
	**Infectious material** This warning symbol indicates the possible existence of biologically dangerous and infectious material. When working with this kind of material always observe the prevailing laboratory safety regulations and take necessary precautions and disinfection measures (e.g. wearing protective clothing, masks, gloves etc.). Non-observance may cause severe personal injury or even death. For information on how to use, dilute and efficiently apply disinfectants, refer to the *Laboratory Biosafety Manual: 2004 by WHO - World Health Organization*.
	**Radioactive material** This warning symbol indicates the possible existence of radioactivity. When working with radioactive material always observe the safety regulations and take necessary protective measures. Wear protective clothing, e.g. masks and gloves. Non-observance may cause severe personal injury or even death.
	**Corrosive substances** This warning symbol indicates the possible existence of corrosive substances. When working with corrosive substances always observe the laboratory safety regulations, and take protective measures (e.g. wear protective masks and gloves). Non-observance may cause severe personal injury or even death.

Waste disposal

Dispose all waste produced (chemicals, infectious and radioactively contaminated substances etc.) according to the prevailing laboratory regulations. Detergents and cleaning agents must be disposed according to the special waste regulations.

1.4 Laser safety

INVENIO S is classified as a laser class 1 product according to IEC/EN 60825-1. Laser class 1 means that the product is incapable of causing eye and skin injuries under normal and reasonably foreseeable conditions of use. Laser radiation is not accessible to the user if the spectrometer is used as intended. The intended use is defined in section 1.5.

 LASER 1 classified according to IEC/EN 60825-1: 2014	This label identifies INVENIO S as a laser class 1 product. It is affixed at the rear side of INVENIO S.
 Complies with 21 CFR 1040.10 and 1040.11 except for deviations pursuant to Laser Notice No. 50, dated June 24, 2007.	The label below indicates that the applied laser standards are accepted in the U.S.

The interferometer is equipped with a semiconductor VCSEL[1] laser diode. This laser emits invisible light with a wavelength of 850 nm. The power output is 2 mW. According to EN 60825-1 (IEC 60825-1), the incorporated laser is laser class 3B product.

1.5 Intended use

INVENIO S is a FTIR spectrometer for analytical applications in the field of research and development. It is designed for FTIR spectroscopic measurements in transmission, reflection, diffuse reflection and ATR. The measurement results can be used for qualitative and quantitative evaluations. The spectrometer is suited for analyzing all kinds of solid, liquid and gaseous samples which absorb infrared light (radiation energy). Special optional accessories allow for sample analysis at temperatures above and below room temperature.

The spectrometer is intended for indoor use only under the environmental conditions specified in appendix A, section A.4.

The intended use includes also the compliance with the relevant standards and regulations, especially:

- regional or national safety regulations
- regional or national accident prevention regulations
- generally recognized technical regulations

The intended use also includes the strict observance of all instructions given in this manual, namely:

- safety instructions
- installation instructions,
- operation instructions
- repair and maintenance instructions

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[1] VCSEL - vertical-cavity surface-emitting laser

➢ **Other use than described above is not intended and can lead injuries and/or property damage.**

⚠ WARNING

Health hazard because of unintended use of the spectrometer

Non-observance of the following safety instruction could result in injury and/or spectrometer damage.

➢ Do not take any actions that violate the intended use. The operational safety of the spectrometer is ensured only if it is used as intended.

Use only components and accessories supplied by Bruker. For components and accessories made by other manufacturers and used in conjunction with the spectrometer, Bruker Optik GmbH does not assume any liability for safe operation and proper functioning.

1.6 Service contact data

In case you have questions about safety, installation and/or operation as well as repair and maintenance of the spectrometer or you need technical assistance in case of a hardware and/or software problem, you can contact the Bruker service as follows:

• Service Hotline Hardware:	+49 (0) 72 43 504-2020
• Service Hotline Software:	+49 (0) 72 43 504-2030
• Fax:	+49 (0) 72 43 504-2100
• E-Mail:	service.bopt.de@bruker.com service.bopt.us@bruker.com

☞ On our website **www.bruker.com/about-us/offices/offices/bruker-optics** you will find also the current contact data of all Bruker Optics service offices worldwide.

2 General

2.1 Technical key features

The FTIR spectrometer INVENIO S is characterized by the following technical key features:

Automatic component and accessory recognition (ACR & AAR)

The spectrometer is equipped with a number of features such as AAR (Automatic Accessory Recognition) and ACR (Automatic Component Recognition) that facilitate performing spectroscopic measurements.

The function **AAR** identifies automatically the QuickLock-type accessory installed in the large-sized sample compartment, performs several tests and loads automatically the corresponding experiment file including the pre-defined measurement parameters.

The function **ACR** recognizes automatically the currently installed optical components such as source and detector. These components are electronically coded so that the spectrometer firmware is able to recognize them. This information is passed on to the application software OPUS. The purpose of ACR is to enable the user to select the right optics parameters in OPUS. In addition, the optical components (e.g. source, laser) are monitored permanently to ensure that they operate within the specification range. This feature is called Performance Guard. Its purpose is to facilitate the system diagnostics in case of an error.

Spectrometer operation by PC (standard) and/or integrated touch panel PC (optional)

By default, the spectrometer is controlled by a data system (e.g. PC workstation, notebook) on which the operating system Microsoft Windows and the spectroscopic software OPUS is installed. The Ethernet connection provides the possibility to control the spectrometer also via your intranet or the Internet. This variant is primarily intended for demanding R&D applications.

Optionally, the spectrometer can be equipped with an integrated panel PC plus touchscreen. The OPUS/TOUCH software, which is especially designed for touchscreen-operation, facilitates standard analytical tasks by simplified workflows and intuitive operation.

Flexible sample compartment concept

By default, the spectrometer has a sample compartment with QuickLock mechanism for positioning QuickLock-type accessories in the sample compartment. For this sample compartment, a large variety of measurement accessories is available. These accessories are designed for dedicated analytical applications.

Optionally, the spectrometer can have a secondary, smaller sized sample compartment with a MIR DTGS detector and a slide bracket which can accommodate different kind of sample accessories (e.g. pellet holder, liquid cell etc). If measurements in the mid IR range are required from time to time, the secondary sample compartment can be used so that sophisticated hardware setups in the main sample compartment do not need to be removed. So the secondary sample compartment enhances the operating comfort of the spectrometer.

☞ For detailed information about the sample compartments, see section 4.1.2.

2.2 Spectrometer variants

INVENIO S is available in different variants which differ from each other in terms of the installed optical components beamsplitter, detector and sample compartment window material. The variants are available only ex factory.

2.2.1 Standard variant

The standard spectrometer variant is designed for spectroscopic measurements in the mid-infrared region only.

Variant	Spectral range	Source	Beamsplitter	Window material	Detector
INVENIO S with standard KBr beamsplitter	8,000 - 340cm^{-1}	MIR source (globar)	KBr (standard)	KBr	DLaTGS[a] with KBr window

a. DLaTGS detector - deuterated L-alanine doped triglycene sulphate detector

In addition to the standard detector, several optional MIR detectors are available. These detectors differ from each other in terms of detection sensitivity and the spectral range, they cover.

☞ The available detectors are listed in section 4.5.3.

☞ For information about how to exchange the detector, see section 5.9.

2.2.2 Optional variants

The following optional spectrometer variants are available:

Variant	Spectral range	Source	Beamsplitter	Window material	Detector[a]
INVENIO S with KBr broad band beamsplitter	11,000 - 350cm^{-1}	for MIR measurements: MIR source (globar) for NIR measurements: NIR source	KBr (broad band)	KBr	for measurements in the MIR range: DLaTGS for measurement in the NIR range: NIR detectors
INVENIO S with CsI optics	5,000 - 200cm^{-1}	MIR source (globar)	CsI	CsI	DLaTGS with CsI window
high humidity variant with ZnSe optics	6,000 - 500cm^{-1}	MIR source (globar)	ZnSe	ZnSe	DLaTGS with KBr window

a. Several optional detectors are available. These detectors differ from each other in terms of detection sensitivity and the spectral range, they cover. See section 4.5.3. For information about how to exchange the detector, see section 5.9.

Spectrometer variant with KBr broad band beamsplitter

With this optional variant, spectroscopic measurements in both the MIR and the NIR region are possible. The extension to the NIR region requires the installation of a NIR source and of a NIR detector.

Note: The NIR source is a factory-installed option. A NIR detector can be installed by the user.

☞ The available detectors are listed in section 4.5.3. For information about how to exchange the detector, see section 5.9.

Spectrometer variant with CsI optics

This optional variant is designed for spectroscopic measurements in both the MIR and the FIR region without the need for exchanging any optical spectrometer component.

NOTE

➢ Cesium Iodide (CsI) is a very hygroscopic material. For this reason, **do not install the spectrometer in a location with a high atmospheric humidity!** Otherwise, the IR-transparency of the optical material (CsI) of the beamsplitter, the detector and the sample compartment window will be reduced within a relatively short period of time to such an extend that the spectrometer does not perform as specified any longer.

High humidity variant with ZnSe optics

This optional variant is especially designed for operating the spectrometer in locations with high atmospheric humidity. The suitability for this special operating condition is achieved by using non-hygroscopic material ZnSe as optical material for the beamsplitter and the sample compartment windows.

2.3 Purge ability

The large-sized sample compartment and the optics of the spectrometer are purgeable. Purging the spectrometer with dry air or nitrogen gas reduces the content of unwanted atmospheric interferents (e.g. water vapor and carbon dioxide) inside the spectrometer significantly. Residual absorption by these atmospheric gases can lead to a significant high noise level and may mask in the IR spectrum weak spectral features of the sample. Purging is the most common method of reducing the water vapor content inside the spectrometer.

☞ For detailed information about purging the spectrometer, see section 5.8.

2.4 Spectrometer validation

The spectrometer and the spectroscopy software OPUS are designed for validating the spectrometer to ensure that the spectrometer operates within the specifications and delivers reliable measurement results. For this purpose, the spectrometer is equipped with a computer-controlled internal validation unit (IVU) as a standard feature. The IVU is a wheel equipped with different standards (test samples) used for validating and testing the instrument performance. Depending on which test protocol (OQ[1] or PQ[2]) is running, the corresponding test sample is moved automatically in the beam path. Validation intervals and test protocols (OQ and PQ) are defined by the user using OVP[3].

☞ For detailed information about OVP and spectrometer validation, refer to the OPUS Reference Manual. I

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[1] OQ - Operational Qualification

[2] PQ - Performance Qualification

[3] OVP - OPUS Validation Program

2.5 Measurement accessories

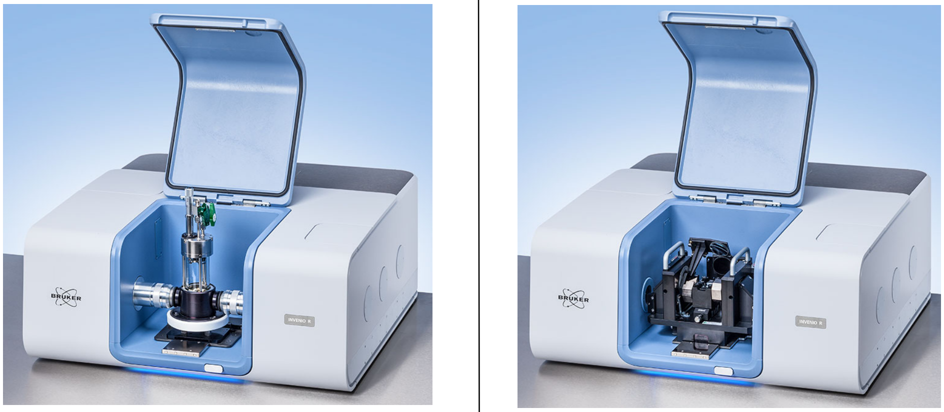
The large-sized sample compartment is equipped with a QuickLock locking mechanism which allows an exact and reproducible positioning of the measurement accessories in this sample compartment.

Bruker offers a large variety of QuickLock-type accessories which are designed for dedicated applications. For example:

- accessories for ATR, transmission, diffuse and specular reflectance spectroscopy
- accessories for variable angle specular reflectance spectroscopy
- liquid cells
- gas cells with variable and fixed path length
- photo-acoustic cell
- automatic sample changers

INVENIO S with AquaSpec cell

INVENIO S with BioATR II unit



INVENIO S with gas cell

INVENIO S with variable angle reflection unit

Figure 2.1: INVENIO S with different QuickLock-type accessories installed in the large-sized sample compartment

☞ For detailed information about the QuickLock mechanism, see section 5.4.

2.6 Possible instrumental set-ups

The spectrometer has three IR beam outlet ports (two outlet ports on the right side and one outlet port on the left side) allowing the connection of a multitude of optional accessories and/or components like:

- HYPERION 1000/2000 IR microscope and HYPERION 3000 imaging microscope with FPA detector (Focal Plane Array detector system)
- HTS-XT module (High Throughput Screening Extension)
- coupling of TGA[1] and GC[2] instruments
- Fiber optic coupling module with MIR or NIR fiber probes for solid and liquid samples

Depending on the requirements, the R&D applications impose on the analysis system, a large number of different instrumental set-ups is possible.

	FT IR microscope of the HYPERION series coupled to the left side and a HTS-XT module coupled to the right side of INVENIO S
	TGA-IR unit plus NETZSCH thermo balance coupled to the right side of INVENIO S

Figure 2.2: Examples of possible instrumental set-ups

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[1] TGA - Thermogravimetric Analysis

[2] GC - Gas Chromatography

2.7 INVENIO S with integrated ATR unit (option)

Figure 2.3: INVENIO S with integrated ATR unit

Optionally, INVENIO S has an integrated ATR unit. The following ATR unit variants are available:

- ATR unit with exchangeable crystal plate (crystal plate with integrated diamond crystal or Germanium crystal)
- ATR unit with a diamond ATR crystal only, heatable
- ATR unit with a diamond ATR crystal only, high-pressure variant

Fields of application

The integrated ATR unit is designed for spectroscopic measurements in attenuated total reflection (ATR). The heatable variant allows for measurements at temperatures up to max. 80°C. The ATR measurement technique is ideal especially for strongly absorbing or thick samples which totally absorb the IR-radiation when measured in transmittance due to their high absorptivity.

The accessory is suitable for measuring the following kinds of samples:

- Liquids (e.g. aqueous solutions)
- Solids (e.g. polymers)
- Powders
- Pastes, gels and creams
- Films
- Surface coatings

➢ **Important:** The sample thickness should not exceed 20 mm.

Technical features

Depending on the variant, the ATR unit is characterized by the following key features:

ATR unit with exchangeable crystal plate	• Diamond and Germanium ATR crystal, single reflection • Ergonomic one-finger clamp mechanism with pressure control • Adjustable and reproducible sample pressure • Sealed and purgeable beam path
heatable ATR unit	• Diamond ATR crystal, single reflection • Ergonomic one-finger clamp mechanism with pressure control • Adjustable and reproducible sample pressure • Heatable crystal plate up to 80°C • Sealed and purgeable beam path
ATR unit, high-pressure variant	• Diamond ATR crystal, single reflection • High-pressure variant with slip clutch high-pressure applicator • Sealed and purgeable beam path

ATR measurement technique - Functional principle

In FTIR spectroscopy, ATR stands for Attenuated Total Reflection and is a special reflection measurement technique. When a sample is measured in ATR, the infrared beam enters the ATR crystal (a prism) that is made of an IR-transparent material and has a high refraction index (e.g. diamond). Due to the internal reflection, the infrared beam reflects off at the crystal surface inside the ATR crystal, at least once before exiting the ATR crystal. (Note: In case of the ATR unit, the IR beam is internally reflected one time.) As a result of the internal reflection, the infrared radiation sets up an evanescent wave which penetrates the sample typically a few micrometers. (Note: For this reason, the sample must be in intimate contact with the ATR crystal.)

The penetrating evanescent wave interacts with the sample, i.e. the sample absorbs energy of the evanescent wave of those wave numbers which are characteristic of the sample in question. Consequently, this absorbed amount of energy is missing in the reflected IR beam. The result of an ATR measurement is an absorption spectrum which shows the intensity change of the reflected IR beam as a function of the wavenumbers.

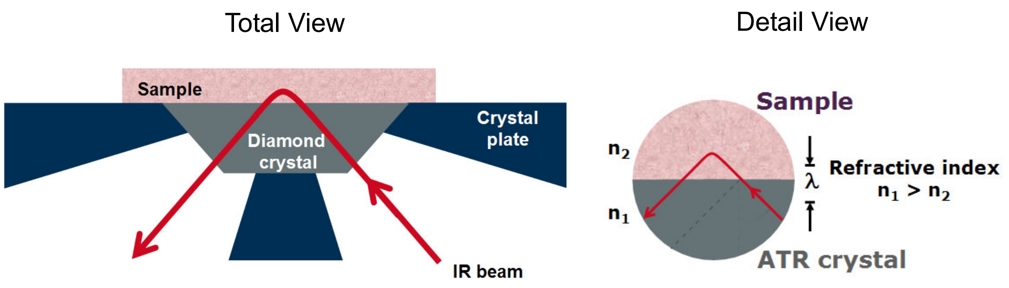


Figure 2.4: Schematic presentation of the IR-beam path in the ATR crystal

The following factors have an influence of the quality of the ATR measurement result:

- the contact between sample and ATR crystal (In case of solid samples, an intimate contact between sample and ATR crystal can be achieved by pressing the sample against the ATR crystal using the pressure application device.)
- the refraction index of the ATR crystal and the refraction index of the sample
- the wavelength of the infrared radiation
- the angle with which the infrared beam enters the ATR crystal

The spectra acquired with the ATR measurement technique are comparable with those spectra measured in transmittance. In case of an ATR spectrum, however, the absorption intensity of the spectral features is lower than in case of the corresponding transmission spectrum, especially in the high-wavenumber region (short wavelength). The reason for this is that the absorption intensity strongly depends on the penetration depth of the evanescent wave into the sample. The penetration depth of the evanescent wave in turn depends on the refraction indices of the sample and the ATR crystal, the contact between sample and ATR crystal as well as the wavelength of the infrared radiation.

Advantages of the ATR measurement technique

- ATR is an non-destructive analysis method, i.e. the sample does not need to be destroyed for the purpose of analyzing.
- Usually, sample preparation is not required.
- The ATR measurement technique requires only a small amount of sample material.
- The ATR measurement technique is also suitable for thick and strongly absorbing samples which cannot be measured in transmission.

Aspects of the ATR measurement technique that require special attention

- In case of a solid sample, the quality of the measurement results depends strongly on the contact pressure with which the sample has been pressed against the ATR crystal during the measurement.
- In case of multi-layer samples, only the outer layer (ca. 2 µm) will be spectroscopically analyzed.
- Possibly existing contaminations (e.g. residuals of the previous sample and/or cleaning agent, fingerprints on the ATR crystal etc.) may falsify the measurement result.

3 Installation

3.1 General information

Installation and initial start-up of the spectrometer are done by Bruker service technicians. The operating company has to provide an installation site that meets the site requirements described in section 3.5. See also the technical document *Installation Requirements for INVENIO S* provided by Bruker Optik GmbH in advance.

The installation of the spectrometer includes the following works:

- connecting the spectrometer to the power supply
- connecting the spectrometer to the purge gas supply line
- connecting the spectrometer to a computer

☞ For detailed information about how to install the computer, refer to the computer manual.

3.2 Delivery scope

The following basic hardware and software items are included in the delivery scope:

Basic hardware components	• INVENIO S spectrometer with standard KBr optics (including the user manual) • External power supply unit with low-voltage cable, power cord with country-specific plug • PC (if desired, the PC can also be provided by the customer) • Data cable (Category 5, crossover cable for 10Base-T Ethernet standard) • Tools and spare parts kit: 1x TORX screw driver (Tx20), 1x special tool for removing / installing a window and flange, 1x container with desiccant, 1x IR sensor card, several sample preparation tools like spatula, tweezers, scalpels etc.)
Standard software	• OPUS software, basic IR package • BPAD spectra library (containing polymer spectra measured with the ATR unit)

The following optional hardware and software items can be included:

Optional hardware components and features	• Optional QuickLock-type measurement accessories • a second, small-sized sample compartment plus measurement accessories designed for this sample compartment • an additional detector position for installing a DigiTect-type detector plus optional DigiTect-type detectors (e.g. MCT) • Integrated touch panel PC • wireless keyboard and mouse for operating the integrated touch panel PC • aluminum mirrors instead of gold mirrors (in preparation for the spectral range extension to UV/VIS) • optical configurations for spectral range extensions to FIR or NIR, or for operation in a high humidity environment • Air flow regulator for the purge gas
Optional software	• Optional OPUS software packages (e.g. OPUS/SEARCH) • OPUS/TOUCH software (only if the optional touch panel PC or a tablet PC is included in the delivery scope) • optional spectra libraries (for special types of material, e.g. chemicals, pharmaceuticals, polymers etc.)

Moreover, Bruker offers also predefined INVENIO S packages for dedicated applications. In the table below, the delivery scope of these packages is listed:

INV-S/STND	**The Standard Package includes:** • INVENIO S spectrometer with standard KBr optics including user manual and all required hardware components (e.g. external power supply unit, cables, tools and spare parts kit) • Integrated touch panel PC • Platinum ATR unit • OPUS/TOUCH software (for operating INVENIO S via touch panel PC) • BPAD spectra library (containing polymer spectra measured with an ATR unit) ➢ Note: In addition, optional hardware components and features as well as optional OPUS software packages and spectra libraries can be included in the delivery scope of the Standard Package. For optional hardware and software items, see table above.
INV-S/MULTI	**The Multi-Purpose Package includes:** • INVENIO S spectrometer with standard KBr optics including user manual and all required hardware components (e.g. external power supply unit, cables, tools and spare parts kit) • Integrated touch panel PC • OPUS/TOUCH software (for operating INVENIO S via touch panel PC) • Integrated Platinum ATR unit • a second, small-sized sample compartment • BPAD spectra library (containing polymer spectra measured with an ATR unit) ➢ Note: In addition, optional hardware components and features as well as optional OPUS software packages and spectra libraries can be included in the delivery scope of the Multi-Purpose Package. For optional hardware and software items, see table above.
INV-S/POLY	**The Polymer Package includes:** • INVENIO S spectrometer with standard KBr optics including user manual and all required hardware components (e.g. external power supply unit, cables, tools and spare parts kit) • Integrated touch panel PC • OPUS/TOUCH software (for operating INVENIO S via touch panel PC) • Integrated Platinum ATR unit, high-pressure variant • BPAD spectra library (containing polymer spectra measured with an ATR) • B-KIMW (Spectra library containing a huge number of high-quality ATR spectra of plastic materials, technical biopolymers and additives) ➢ Note: In addition, optional hardware components and features as well as optional OPUS software packages and spectra libraries can be included in the delivery scope of the Polymer Package. For optional hardware and software items, see table above.

INV-S/PROT	**The Protein Analysis Package includes:** • INVENIO S spectrometer with standard KBr optics including user manual and all required hardware components (e.g. external power supply unit, cables, tools and spare parts kit) • an additional detector position for installing a DigiTect-type detector (e.g. MCT) • Air flow regulator (for regulating the purge gas flow rate) • AquaSpec unit • Bio-ATR II unit • Thermostat (temperature range: -25°C to 150°C) • OPUS/PRO software package • OPUS/3D software package • BPAD spectra library (containing polymer spectra measured with the ATR) ➢ A photovoltaic MCT detector is required which is not included in this package. **The following optional items and features can be included the delivery scope of this package:** • BQG - Protein spectra library (spectra of proteins in aqueous solution, measured with AquaSpec cell) • B-PROT1 - Calibration for protein secondary structure analysis, based on AquaSpec data • B-PROT2 - Calibration for protein determination, based on AquaSpec data • Spare filter set for AquaSpec cell (2µm) • Injection ports for AquaSpec cell • ProteoClean10 - kit for cleaning of the AquaSpec cell from adsorbed protein • CellProtect 5 - Disinfection and storage solution for the AquaSpec cell • Pumping valve for N2 detector-dewars
INV-S/PHA	**The Pharma Package includes:** • INVENIO S spectrometer with standard KBr optics including user manual and all required hardware components (e.g. external power supply unit, cables, tools and spare parts kit) • Integrated touch panel PC • OPUS/TOUCH software (for operating INVENIO S via touch panel PC) • Integrated Platinum ATR unit • a second, small-sized sample compartment • BPAD spectra library (containing polymer spectra measured with an ATR unit) **Included validation features:** • System Validation Manual • OPUS/VALIDATION software package • Internal Validation Unit (IVU) with reference standards for automated instrument tests for operational and performance qualification (OQ and PQ) • Certified reference material Polystyrene BRM1921 integrated in the IVU, used for automated instrument test routines according to the European Pharmacopoeia, Chapter 2.2.24., Japanese Pharmacopoeia 2.25. and USP <854>. • O/PHEUR 2224 plug-in module ➢ Note: In addition, optional hardware components and features as well as optional OPUS software packages and spectra libraries can be included in the delivery scope of the Pharma Package. For optional hardware and software items, see table above.

3.3 Inspecting the packaging

After having received the spectrometer, inspect the packaging for damages.

⚠ CAUTION

Possible damage to the delivered spectrometer because of transport damage

Non-observance of the following safety instructions could result in injury.

- ➢ Inspect the packaging for damages. If there are signs of damage contact shipping company.
- ➢ A spectrometer delivered in a damaged packaging may be damaged as well. Therefore, in this case do not put the spectrometer into operation. Contact Bruker instead. (For the contact data, see section 1.6.)

3.4 Transporting the spectrometer

The spectrometer has to be carried by at least two persons. Due to the spectrometer weight (ca. 65 kg), this method of transport is suited only for very short distances. **Attention:** To carry the spectrometer by hand, **first remove the magnetically fixed slats at the bottom of the left and right spectrometer side!**

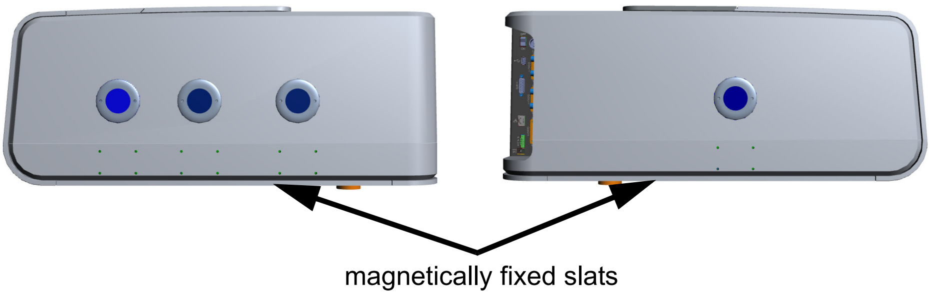


Figure 3.1: Location of the slats

For transporting the spectrometer over longer distances, it is recommended to use a wheeled table, for example.

⚠ CAUTION

Injury and/or spectrometer damage due to an inadequate method of transport

Non-observance of the following safety instructions could result in injury.

- ➢ For short-distance transport, the spectrometer has to be carried by at least two persons. But pay attention to the spectrometer weight (ca. 65 kg).
- ➢ For long-distance transport, put the spectrometer on a wheeled table or use a fork lifter, for example. To avoid damages, transporting the spectrometer in original packing is recommended.

3.5 Site requirements

The operating company has to provide an installation site that meets the following site requirements:

Space requirements:	• Floor space: 80 cm x 80 cm • Height without panel PC and touch screen: 32 cm • Height with panel PC and touch screen: 50 cm • Height with open sample compartment: 62 cm ☞ For exact spectrometer dimensions refer to appendix D. • At the rear side, the spectrometer requires a clearance of at least 15 cm. • Place the spectrometer on a stable and horizontal base which is rated for the weight of the complete system. The spectrometer (the basic instrument) has a weight of about 65 kg. Additional accessories increase the weight correspondingly.
Environmental conditions:	• Ambient temperature range: 18°C - 35°C • Ambient temperature variations: max. 1°C/h and max. 2°C/day (Temperature variations can impair the results of long-term measurements.) • Humidity (non-condensing): ≤ 80% (relative humidity) • Installation site: in a closed room, max. 2000 m above sea level • The spectrometer should not be installed near vibration sources (e.g. ventilation hoods, air conditioners, motors, elevators) or in rooms with intense floor vibrations. • The spectrometer should not be installed near sources of potential inductive electrical interference (e.g. pumps, switching motors, microwave ovens etc.), sources of high energy pulses, and sources that might cause magnetic or radio frequency interference. These devices can interfere with the spectrometer and cause spectrometer malfunction. Ensure that these types of devices are not connected to the same electrical circuit as the spectrometer.
Purge gas supply requirements:	• dry air or nitrogen gas (dew point < -40°C corresponds to a degree of dryness of 128 ppm humidity) • oil-free and dust-free (Recommendation: Use of DIN purity class 1-1-1 (dryness - residual oil - particles) • max. pressure: 0.5 bar (7.25 psi) overpressure • Recommended purge gas flow rate: 200 liters/hour. • Purge gas flow rate must not exceed 500 liters/hour. Note: The local purge gas supply line needs to be dimensioned for a PVC hose having an outer diameter of 6 mm. ℹ For regulating the purge gas flow rate, an air flow regulator (order no: S316/7) is optional available.

Power supply requirements:	The spectrometer power supply is realized by the supplied external power supply unit. The external power supply unit has a wide input range which means that it is able to adapt itself to the most common public supply mains. • Input range: 100 - 240 V AC, 2.5 A max., 50- 60 Hz • Output: 24 V DC, 3.75 A Connect the spectrometer only to a socket outlet with earthing contact that complies with VDE 0620-1 or IEC! The spectrometer is constructed for the connection to a SELV (safety extra low voltage) circuit. For safety reasons, make sure that the interfaces of electric accessories connected to the spectrometer comply with SELV (safety extra low voltage) circuit requirements. Normally, this condition is met if the accessory design is based on the requirements described in EN 61010 or EN 60950. If there are problems concerning main power supply (e.g. brownouts, power surges, frequent thunderstorms or power blackouts) use an UPS unit (Uninterruptible Power Supply) to ensure an uninterruptible power supply and consequently an operation without interruptions.
Possibilities of interrupting the mains power supply:	The mains power supply of the spectrometer can be interrupted as follows: • by pulling the mains plug of the power cord • by switching off the spectrometer using the ON / OFF switch at the spectrometer rear side ➢ Ensure that the wall socket and the ON/OFF switch at the spectrometer rear side are easily accessible at any time in order to be able to interrupt the power supply without any hindrance.
External devices:	• Line-powered accessories connected to spectrometer interfaces (e.g. Ethernet) have to have special electrical disconnecting features. The electric circuits of these interfaces have to comply with the requirements imposed on SELV circuits (safety extra low voltage circuit). ℹ Typically, this is achieved when connecting SELV circuits to each other. In general, the interface meets the requirement if the device complies with the regulations outlines in EN 61010 (Safety regulations for laboratory equipment) or EN 60950 (Safety for information technology facilities).

3.6 Connecting the spectrometer to the power supply

3.6.1 General information

The spectrometer power supply is realized by an external power supply unit. The external power supply unit plus power cord and low-voltage cable are included in the standard delivery scope of the spectrometer.

The external power supply unit has a wide input range which means that it is able to adapt itself to the most common public supply mains.

- Input range: 100 - 240 V AC, 2.5 A max, 50- 60 Hz
- Output: 24 V DC, 3.75A

Depending on the local conditions, the original power cord may need to be exchanged for a power cord that complies with the standards of the country in question. Ensure that the installed power cord has the approval of the local authority (UL for US, CSA for Canada or VDE for Europe).

3.6.2 Safety note

To ensure a safe operation of the external power supply unit, observe the following safety instructions:

- Operate the external power supply unit only in a dry environment (20% to 80% relative humidity).
- Make sure that the external power supply unit is not exposed to direct sunlight. During operation, avoid ambient temperatures above +40°C. Provide for sufficient air circulation.
- Do not place the external power supply unit on a hot surface.
- Position the external power supply unit in such a way that it does not present a trip hazard.
- Do not put heavy objects on the external power supply unit.

WARNING

Electric shock hazard because of power supply unit damage or unauthorized repair

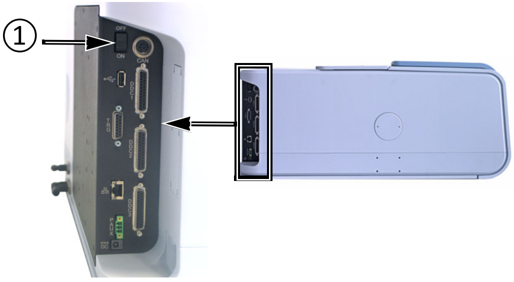
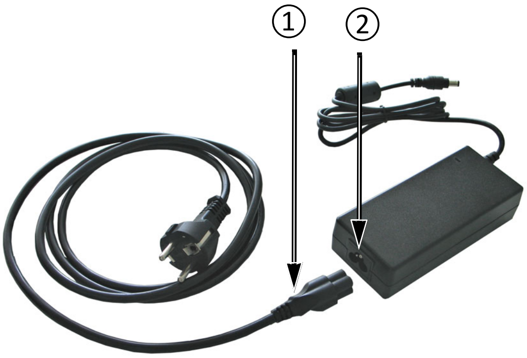
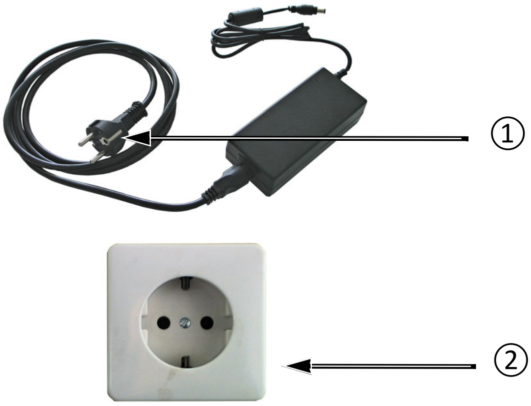
Non-observance of the following safety instructions could result in health problems.

➢ If the external power supply unit and/or the power cord are damaged disconnect the power supply unit instantly from the supply circuit.

➢ Never put a damaged external power supply unit and/or power cord into operation!

➢ Do not try to repair a damaged power supply unit by yourself. Only authorized technicians are allowed to repair the external power supply unit.

3.6.3 Procedure

1		Make sure that the spectrometer is switched off. To do this, check the setting of the ON/OFF switch ①.
2		Connect the power cord ① to the C5 connector of the external power supply unit ②.
3		Connect the low-voltage cable ① to the low-voltage socket ② at the spectrometer rear side.
4		Connect the power plug ① of the power cord to the mains socket outlet ②. **WARNING:** Connect the power cord only to a socket outlet with earthing contact. Make sure that the socket complies with IEC. Otherwise, there is the risk of injury and/or property damage!

3.7 Connecting the spectrometer to the purge gas supply line

3.7.1 General information

The spectrometer has two purge gas inlets; one for purging the sample compartment and the other for purging the optical bench (i.e. interferometer and detector compartment). The purge gas inlets and the purge gas outlet are at the spectrometer rear side.

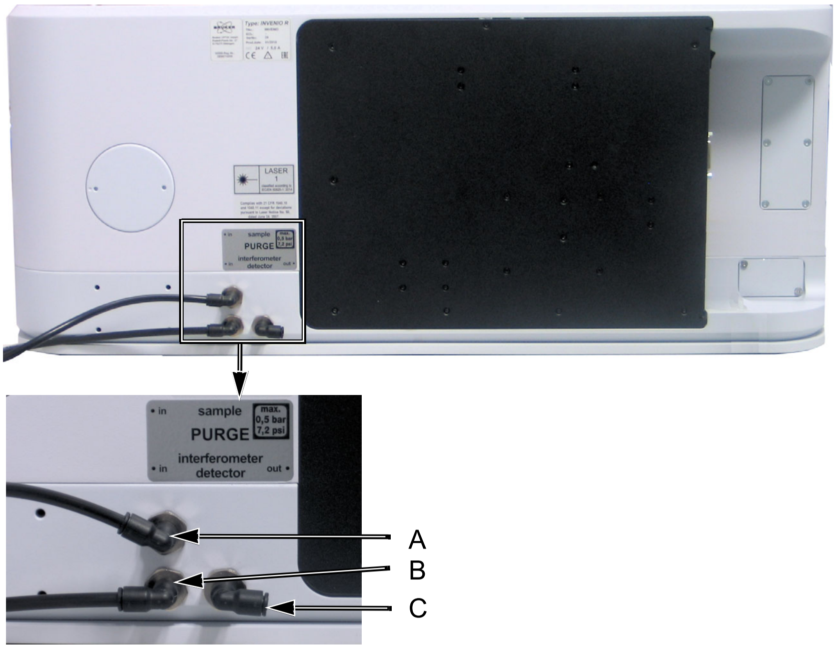


Figure 3.2: Location of the purge gas inlets and outlet (Spectrometer rear side)

Figure 3.2	Purge gas inlet / outlet for ...
A	Purge gas inlet for sample compartment
B	Purge gas inlet for optical bench
C	Purge gas outlet for the optical bench

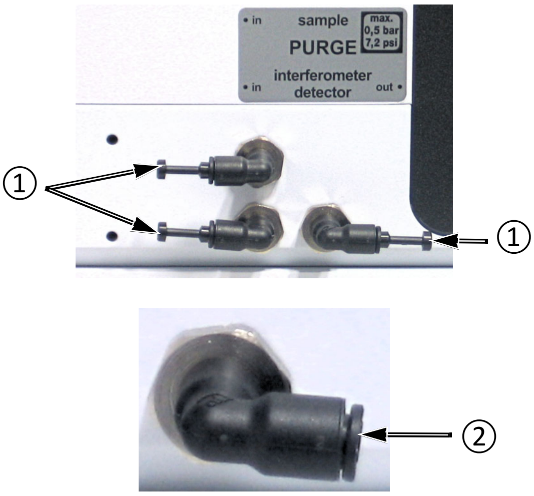
3.7.2 Purge gas supply requirements

The purge gas supply has to meet the following requirements:

- dry air or nitrogen gas (dew point < -40°C corresponds to a degree of dryness of 128ppm humidity)
- oil-free and dust-free
- max. pressure: 0.5 bar (7.25 psi)
- Controllable flow rate (Note: When the spectrometer is purged continuously the recommended flow rate is 200 liters/hour. Make sure that the flow rate does not exceed 500 liters/hour.)

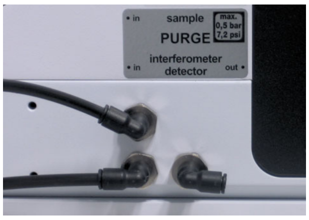
3.7.3 Procedure

The required hoses are not included in the standard delivery scope. Normally, it is the operating company's duty to provide the hoses of the required length (PVC hose, outer diameter: 6mm). Make sure that the hose is rated for the indicated operating pressure. Only in case the purge option S316/7 has been ordered, the required hoses and an air flow regulator are included in the delivery scope of the spectrometer.

<table>
<tr>
<td>1</td>
<td> </td>
<td>Remove the plugs ① from the purge gas inlets and the purge gas outlet.

Note: When you intend to purge the optical bench, do not forget to remove the plug of the purge gas outlet as well. Otherwise, overpressure will build up inside the spectrometer during purging. This may lead to spectrometer damage.

To remove a plug, press the lock ring ② inwards and pull out the plug.

Note: All purge gas ports have such a lock ring. The lock ring prevents the hose from being pulled out unintentionally.</td>
</tr>
<tr>
<td>2</td>
<td> </td>
<td>Insert the hoses into the purge gas inlets.</td>
</tr>
<tr>
<td>4</td>
<td colspan="2">Connect the other end of the hose to the local purge gas supply line. i

It is recommended to install an air flow regulator to ensure a constant air flow of ca. 200 liters/hour. Bruker offers an air flow regulator (purge option S316/7).</td>
</tr>
</table>

Depending on whether you want to purge either only the sample compartment or only the optical bench (i.e. interferometer compartment and detector compartment) or both compartments, there are two variants for connecting the hose.

For purging EITHER the sample compartment OR the optical bench

Required items:

- a stiff PVC hose with an outer diameter of 6 mm

Procedure:

- Remove the plug from the purge gas inlet of either the sample compartment (A in fig. 3.2) or the optical bench (B in fig. 3.2) and insert the hose in the purge gas inlet.
- Connect the other end of the hose to the local purge gas supply line.
- In case the optical bench is purged, remove the plug from the purge gas outlet as well.

For purging BOTH the sample compartment AND the optical bench

Required items:

- a stiff PVC hose (T-shaped) with an outer diameter of 6mm

Procedure:

- Connect the main end of the T-shaped hose to the local purge gas supply line.
- Remove the plugs from both purge gas inlets at the spectrometer rear side (A and B in fig. 3.2) and insert the other two ends of the hose in the purge gas inlets.
- Remove the plug from the purge gas outlet.

3.8 Connecting the spectrometer to a PC

3.8.1 General information

The following table provides a general overview of the possible connection setups.

	**INVENIO S is to be operated only with integrated touch panel PC (optional feature)** In this case, the communication connection between spectrometer and integrated touch panel PC is already factory-installed. No additional connection is required.
	**INVENIO S with or without integrated touch panel PC connected to an external PC** Depending on whether the PC is WLAN-capable or not, the connection setup can be realized in a wired or wireless manner. ☞ For information about the possible connection variants and the installation procedures, see sections 3.8.2.
	**INVENIO S with or without integrated touch panel PC connected to a laptop** Depending on whether the laptop is WLAN-capable or not, the connection setup can be realized in a wired or wireless manner. ☞ For information about the possible connection variants and the installation procedures, see sections 3.8.3.
	**INVENIO S connected to a tablet PC** ☞ For information about the installation procedure, see section 3.8.4.

Depending on the connection setup you want to establish, the following hardware items are required:

- cross-over data cable *
- straight-through data cable (category 5 with RJ45 plugs for Ethernet standard 10/100Base-T) **
- Ethernet hub or Ethernet hub with WLAN **
- LAN USB adapter **
- WLAN stick ***

Note: Normally, PC, laptop and/or tablet are delivered by Bruker. If desired, they can also be provided by the operating company.

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* This item is included in the standard delivery scope of the spectrometer.

** This item needs to be provided by the operating company.

*** If the WLAN stick has not been purchased from Bruker, ensure that it has the following certifications: CE, FCC, NCC. The installation of a WLAN stick provided by the user can be performed by the Windows administrator account.

Figure 3.3 and figure 3.4 illustrate the locations of the Ethernet ports for connecting the data cable(s).

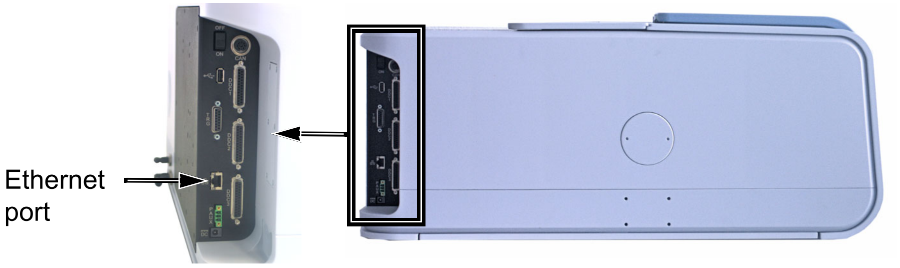


Figure 3.3: Spectrometer - Location of the Ethernet port

Depending on the connection variant, the data cable is connected to different Ethernet ports at the PC.

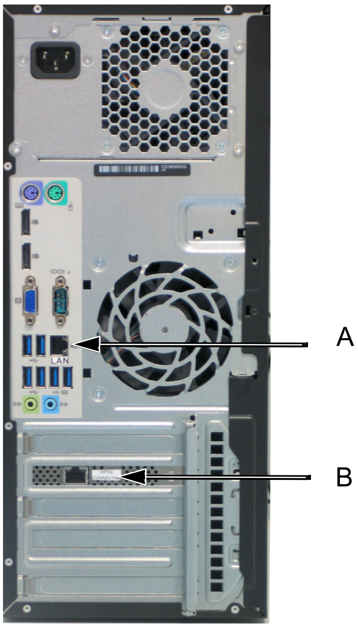


Figure 3.4: PC rear side - Ethernet connectors (in case of a PC supplied by Bruker)

Fig. 3.4	**Ethernet port**
A	labeled LAN **Note:** At this Ethernet port, connect only a straight through data cable.
B	labeled OPTIC CONNECTOR **Note:** At this Ethernet port, connect only a crossover data cable.

Note: The labels OPTIC CONNECTOR and LAN exist only in case of a PC delivered by Bruker.

3.8.2 Possible connection variants for connecting an external PC

Variant A: Connecting the spectrometer to a stand-alone PC

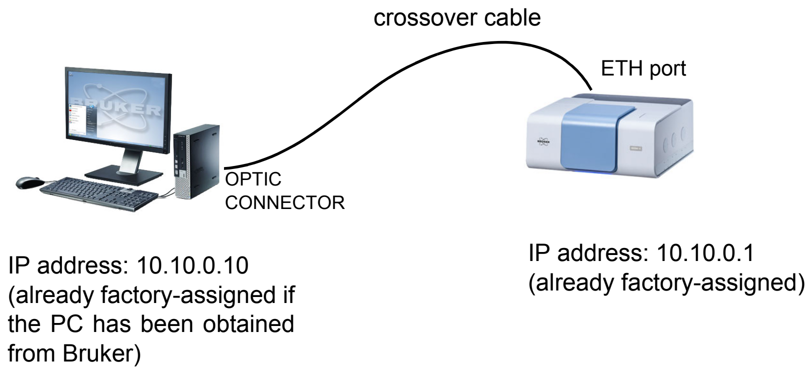


Figure 3.5: Connecting the spectrometer to a stand-alone PC

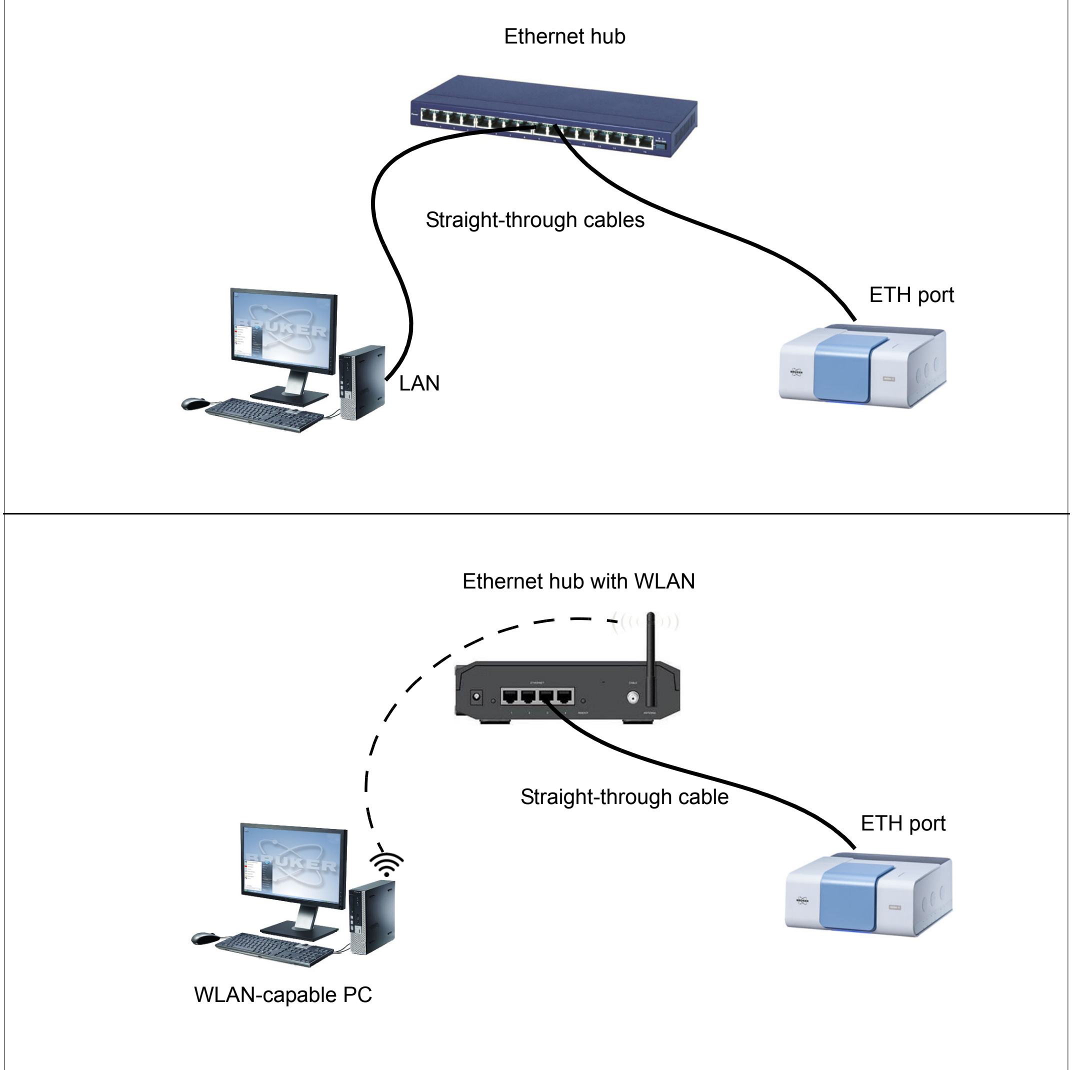
Procedure

1. **Establishing a communication connection between the spectrometer and PC:** Connect the crossover data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the OPTIC CONNECTOR[1] (B in fig. 3.4) at the PC rear side.
2. **IP address assignment:** Only in case the PC has **NOT** been obtained from Bruker, you have to assign the IP address 10.10.0.10 to the PC network card to which the spectrometer is connected. Otherwise, you can skip this step because this IP address is already factory-assigned.
3. **Communication check:** Check the communication between spectrometer and PC. (See section 3.8.7.)

---

[1] Note: The Ethernet ports are labeled only if the PC has been obtained from Bruker.

Variant B: Connecting both spectrometer and PC(s) to a network



Spectrometer and PC require individual IP addresses.
They can be assigned either statically or dynamically.

Note: The integrated touch panel PC, if available, has access to network via the Ethernet connection of the spectrometer.

Figure 3.6: Connecting the spectrometer directly to a network

Procedure

1. **Establishing the connections between the spectrometer and the network**

Connect one straight-through data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the Ethernet hub.

2. **Establishing the connection between the PC and the network**

   - **Wired connection:** Connect the other straight-through data cable to the LAN[1] connector (A in fig. 3.4) at the PC rear side and to the Ethernet hub.
   - **Wireless WLAN connection:** Establish a WLAN connection between the WLAN-capable PC and the WLAN-capable Ethernet hub. Note: The transmission rate must be high (at least 54 Mbit/s).

3. **IP address assignment**

All IP addresses (i.e. IP address of the spectrometer and the PC) can be assigned either dynamically or statically. In the latter case, your network administrator has to define the static IP addresses.

   a) **Spectrometer:** For information about the IP address assignment by DHCP, see section 3.8.6.2. For information about how to assign a static IP address to the spectrometer using the FCONF program, see section 3.8.6.3.

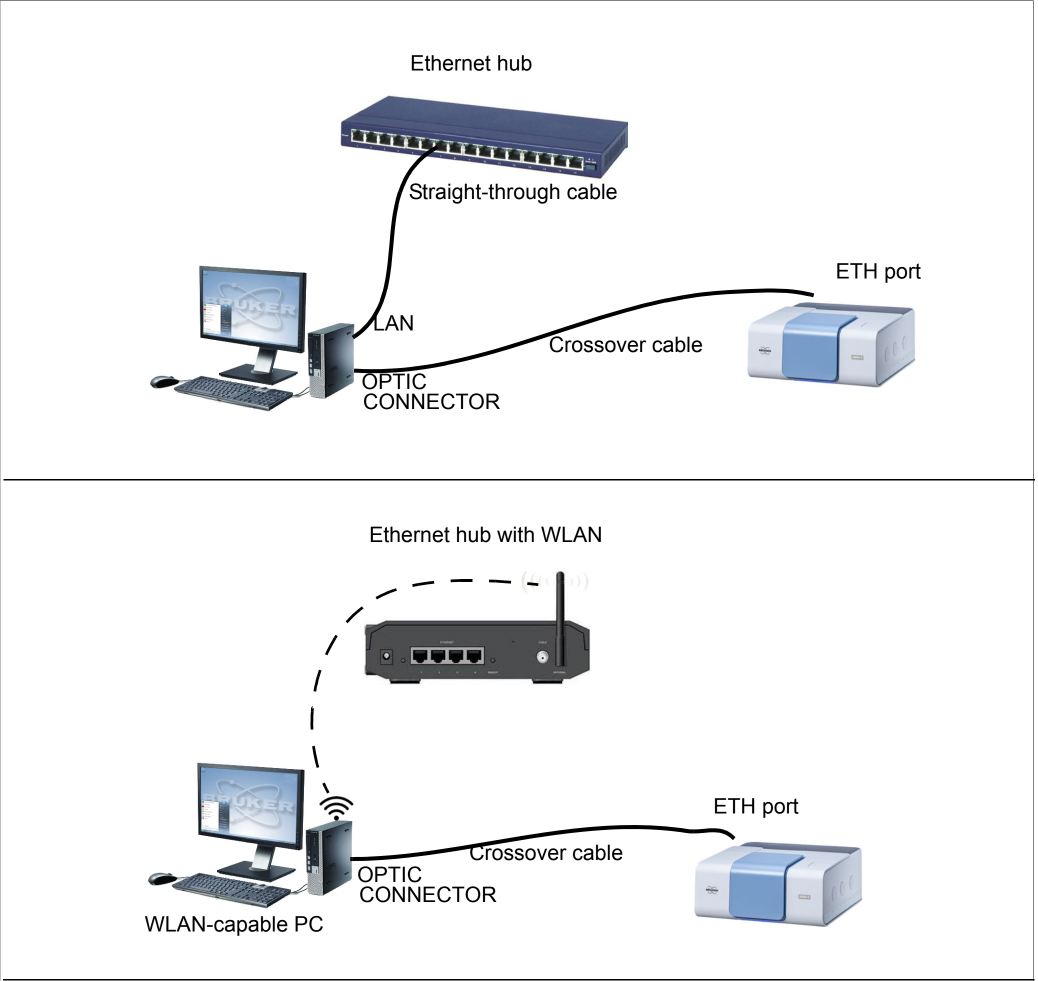
   b) **PC:** The IP address assignment can be either dynamic or static. (For support, contact your network administrator.)

4. **Communication check:** Check the communication between spectrometer and PC. (See section 3.8.7.)

---

[1] Note: The Ethernet ports are labeled only if the PC has been obtained from Bruker.

Variant C: Connecting the spectrometer to a network PC



OPTIC CONNECTOR network card:
IP address: 10.10.0.10
(already factory-assigned if the PC has been obtained from Bruker)

LAN network card:
Either a dynamically assigned IP address or an individual, statically assigned IP address.

IP address: 10.10.0.1
(already factory-assigned)

Figure 3.7: Connecting the spectrometer to a PC which is integrated into a network

Procedure

1. **Establishing a communication connection between the spectrometer and the external PC**
   a) Connect the crossover data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the OPTIC CONNECTOR[1] (B in fig. 3.4) at the PC rear side.

   b) Only in case the PC has **NOT** been obtained from Bruker, you have to assign the IP address 10.10.0.10 to the PC network card to which the spectrometer is connected. Otherwise, you can skip this step because this IP address is already factory-assigned.

   c) Check the communication between spectrometer and PC. (See section 3.8.7.)

2. **Establishing a communication connection between the external PC and the Ethernet hub with or without WLAN**
   a) **wired connection:** Connect the straight-through cable to the LAN[1] connector (A fig. 3.4) at the PC rear side and to an Ethernet hub. (Note: In case the PC is equipped with only one network card, this second communication interface has to be realized by an LAN USB adapter.)

   wireless connection: Establish a WLAN connection between the WLAN-capable PC and the WLAN-capable Ethernet hub. Note: The transmission rate must be high (at least 54 Mbit/s).

   b) Assign an IP addresses to the PC network card to which the Ethernet hub is connected. (Note: In case the PC has been obtained from Bruker, this network card is labeled LAN.) The IP address assignment can be either dynamic or static. (Note: In the latter case, the IP address has to be defined by your network administrator.)

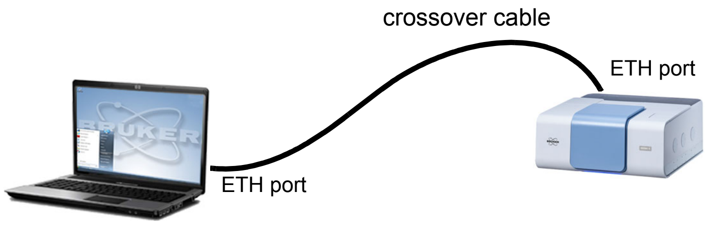
3. **Communication check:** Check the communication between spectrometer and PC. (See section 3.8.7.)

---

[1] Note: The Ethernet ports are labeled only if the PC has been obtained from Bruker.

3.8.3 Possible connection variants for connecting a laptop

Variant A: Connecting the spectrometer to a stand-alone laptop



IP address: 10.10.0.10 (already factory-assigned if the laptop has been obtained from Bruker)

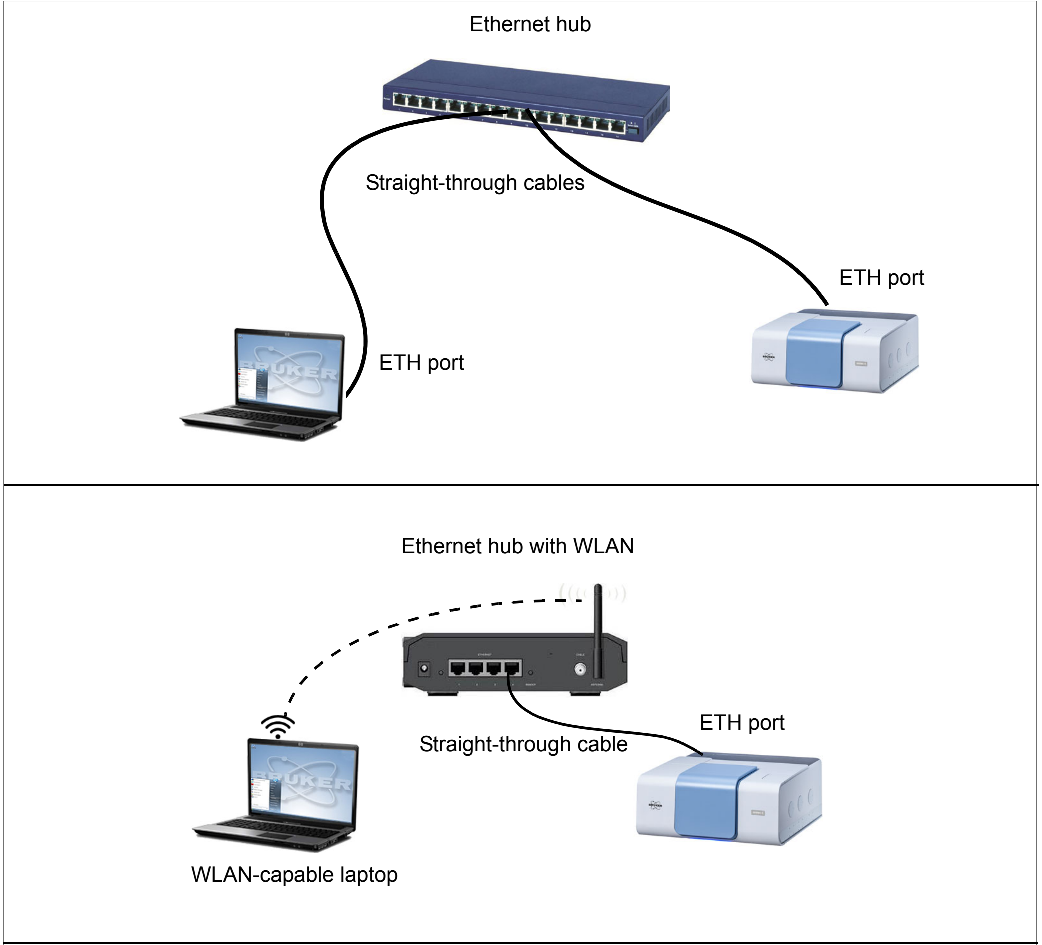
IP address: 10.10.0.1 (already factory-assigned)

Figure 3.8: Connecting the spectrometer directly to a stand-alone laptop

Procedure

1. **Establishing a communication connection between the spectrometer and laptop:** Connect the crossover data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the Ethernet port at the laptop.
2. **IP address assignment:** Only in case the laptop has **NOT** been obtained from Bruker, you have to assign the IP address 10.10.0.10 to the laptop network card to which the spectrometer is connected. Otherwise, you can skip this step because this IP address is already factory-assigned.
3. **Communication check:** Check the communication between spectrometer and laptop. (See section 3.8.7.)

Variant B: Connecting both spectrometer and laptops to a network



**Spectrometer and laptop require individual IP addresses.
They can be assigned either statically or dynamically.**

Note: The integrated touch panel PC, if available, has access to network via the Ethernet connection of the spectrometer.

Figure 3.9: Connecting the spectrometer directly to a network

Procedure

---

1. **Establishing the connection between the spectrometer and the network**

Connect one straight-through data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the Ethernet hub.

2. **Establishing the connection between the laptop and the network**

   - **Wired connection:** Connect the other straight-through data cable to the Ethernet port at the laptop and to the Ethernet hub.
   - **Wireless WLAN connection:** Establish a WLAN connection between the laptop and the WLAN capable Ethernet hub. Note: The transmission rate must be high (at least 54 Mbit/s).

3. **IP address assignment**

All IP addresses (i.e. IP address of the spectrometer and the laptop) can be assigned either dynamically or statically. In the latter case, your network administrator has to define the static IP addresses.

   a) **Spectrometer:** For information about the IP address assignment by DHCP, see section 3.8.6.2. For information about how to assign a static IP address to the spectrometer using the FCONF program, see section 3.8.6.3.

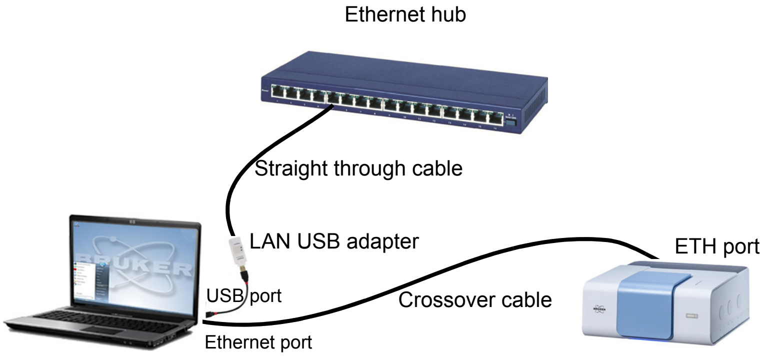
   b) **Laptop:** The IP address assignment can be either dynamic or static. (For support, contact your network administrator.)

4. **Communication check:** Check the communication between spectrometer and laptop. (See section 3.8.7.)

Variant C: Connecting the spectrometer to a network laptop

This connection variant requires two communication interfaces: one interface for the communication between laptop and spectrometer and another interface for the communication between laptop and network. In case of a laptop with only one network card, the second communication interface has to be realized by an LAN USB adapter which has to be connected to the laptop.

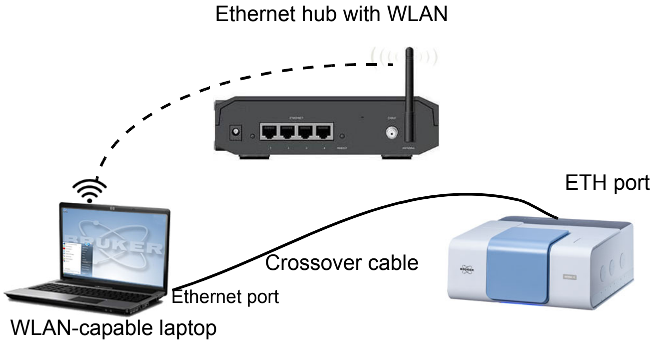
The network card installed in the laptop is used for the communication between laptop and spectrometer. A LAN USB adapter connected to the laptop is used for the communication between laptop and local area network.



Integrated network card:
IP address: 10.10.0.10
(already factory-assigned if the laptop has been obtained from Bruker)

LAN USB adapter:
Either a dynamically assigned IP address or an individual, statically assigned IP address.

IP address: 10.10.0.1
(already factory-assigned)



Integrated network card:
IP address: 10.10.0.10
(already factory-assigned if the laptop has been obtained from Bruker)

WLAN card:
Either a dynamically assigned IP address or an individual, statically assigned IP address.

IP address: 10.10.0.1
(already factory-assigned)

Figure 3.10: Connecting the spectrometer to a laptop which is integrated into a local area network

Procedure

1. **Establishing a communication connection between the spectrometer and the laptop**
    a) Connect the crossover data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the Ethernet port at the laptop rear side.

    b) Only in case the laptop has **NOT** been obtained from Bruker, you have to assign the IP address 10.10.0.10 to the laptop. Otherwise, you can skip this step because this IP address is already factory-assigned.

    c) Check the communication between spectrometer and laptop. (See section 3.8.7.)

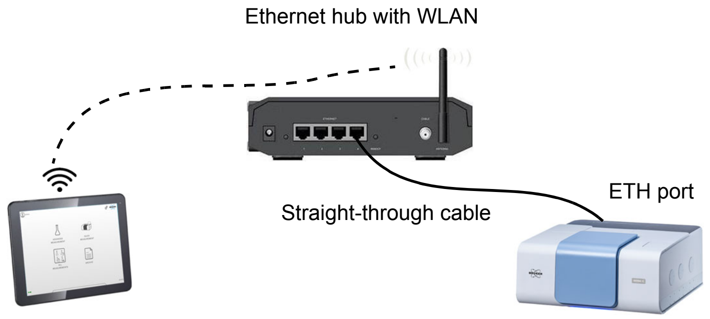
2. **Establishing a communication connection between the laptop and the Ethernet hub**
    a) **wired connection:** Insert the LAN USB adapter into an USB port at the laptop. Connect the straight-through cable to the Ethernet port of the LAN USB adapter and to the Ethernet hub.

    wireless connection: Establish a WLAN connection between the WLAN-capable laptop and the WLAN-capable Ethernet hub. Note: The transmission rate must be high (at least 54 Mbit/s).

    b) Assign an IP addresses to the LAN USB adapter. The IP address assignment can be either dynamic or static. (Note: In the latter case, the IP address has to be defined by your network administrator.)

3. **Communication check:** Check the communication between spectrometer and laptop. (See section 3.8.7.)

3.8.4 Connecting a tablet PC



Spectrometer and tablet PC require individual IP addresses. They can be assigned either statically or dynamically.

Figure 3.11: Connecting the spectrometer to a tablet PC

Procedure

1. **Establishing the connection between the spectrometer and the network**
    - Connect one straight-through data cable to the Ethernet port at the spectrometer rear side (A in fig. 3.3) and to the Ethernet hub.
2. **Establishing the connection between the tablet PC and the WLAN network**
    - Establish a WLAN connection between the tablet PC and the WLAN capable Ethernet hub. Note: The transmission rate must be high (at least 54 Mbit/s).
3. **IP address assignment**

All IP addresses (i.e. IP address of the spectrometer and the tablet PC) can be assigned either dynamically or statically. In the latter case, your network administrator has to define the static IP addresses.

a) **Spectrometer:** For information about the IP address assignment by DHCP, see section 3.8.6.2. For information about how to assign a static IP address to the spectrometer using the FCONF program, see section 3.8.6.3.

b) **Tablet PC:** The IP address assignment can be either dynamic or static. (For support, contact your network administrator.)

4. **Communication check:** Check the communication between spectrometer and laptop. (See section 3.8.7.)

3.8.5 Network addresses

The possible connection variants require different network addresses for spectrometer and PC.

Network addresses in case of connection variant A (i.e. connecting the spectrometer to a stand-alone computer):

The spectrometer and the PC delivered by Bruker are factory-configured for the stand-alone operation as follows:

	Spectrometer	**PC (OPTIC CONNECTOR network card)**	**Note**
IP address	10.10.0.1	10.10.0.10	--
Subnet mask	255.255.255.0	255.255.255.240	--
Gateway	0.0.0.0	0.0.0.0	Do not define in case of Windows XP.

➢ In case **the computer has been obtained from Bruker**, all network addresses are already factory-assigned.

➢ In case **the computer has been provided by the operator**, your network administrator has to assign the network address to the network card installed in the PC. The network address for the network card installed in the PC is listed in the above table.

Network addresses in case of connection variant B (i.e. connecting both computer and spectrometer directly to a network):

In case of this connection variant, an individual IP address needs to be assigned to the spectrometer. An IP address can be assigned to the spectrometer either by DHCP or using the FCONF program. In case a static IP address or a static DHCP (DHCP reservation) is desired, the network administrator has to define the IP address of the spectrometer and all PCs involved because the IP addresses depend on the local intranet.

- Spectrometer and PC(s) must have an unique IP address each. **Important: A wrong IP address can cause problems with other devices connected to the network!**
- In case the PC has been obtained from Bruker, the network address has to be assigned to the LAN network card of the PC.
- In case the spectrometer is to be accessed via Internet, you have to specify a gateway address as well. Note: The gateway links your intranet domain to other domains (e.g. domains being part of the Internet).
- In case the spectrometer is not to be accessed via Internet, set the gateway address to 0.0.0.0.
- In case of the operating system Windows XP, do not specify a gateway.

☞ For information about how to assign a network address to the spectrometer, see section 3.8.6.

Network addresses in case of connection variant C (i.e. connecting the spectrometer to a network computer):

The implementation of this connection variant requires three sets of network addresses:

- one set of network addresses for the spectrometer
- one set of network addresses for the network card in the PC for the communication between PC and spectrometer
- one set of network addresses for the network card in the PC or the USB LAN adapter connected to the PC for the communication between PC and network

➢ In case **the computer has been obtained from Bruker**, the network address for the communication between computer and spectrometer is already assigned. The network address for the communication between computer and network needs to be defined and assigned by your network administrator.

➢ In case **the computer has been provided by the operator**, your network administrator has to assign both the network address for the communication between computer and spectrometer and the network address for the communication between computer and network. The network address for the communication between computer and spectrometer is listed in the above table.

PC with two network cards obtained from Bruker

In case the PC has been obtained from Bruker, it is equipped with two network interface cards labeled OPTIC CONNECTOR and LAN. The network address of the OPTIC CONNECTOR is already factory-assigned for the communication between PC and spectrometer. The network address of the LAN network card needs to be defined and assigned by your network administrator. It is the network card for the communication between PC and network.

	Spectrometer	**OPTIC CONNECTOR network card**	**LAN network card**
IP address	10.10.0.1	10.10.0.10	defined by network administrator or DHCP
Subnet mask	255.255.255.0	255.255.255.240	defined by network administrator
Gateway	0.0.0.0 Do not define in case of Windows XP.	0.0.0.0 Do not define in case of Windows XP.	defined by network administrator

PC with one network card

In case of a PC with only one network card, a LAN USB adapter is required. The network card installed in the PC has to be used for the communication between PC and spectrometer. The LAN USB adapter is used for the communication between PC and network.

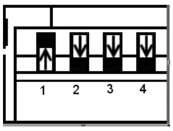
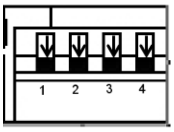
	Spectrometer	**network card installed in the PC**	**LAN USB adapter**
IP address	10.10.0.1	10.10.0.10	defined by network administrator or DHCP
Subnet mask	255.255.255.0	255.255.255.240	defined by network administrator
Gateway	0.0.0.0 Do not define in case of Windows XP.	0.0.0.0 Do not define in case of Windows XP.	defined by network administrator

3.8.6 Assigning an IP address to the spectrometer

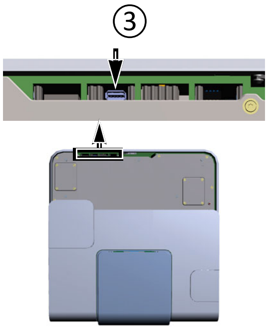
3.8.6.1 General information

By default, the spectrometer is delivered with the factory-assigned standard IP address 10.10.0.1. In case of connection variant A and C, there is no need for assigning a different IP address to the spectrometer. Only in case of connection variant B (i.e. connecting the spectrometer directly to a network, see fig. 3.6), a different spectrometer IP address is required. An IP address can be assigned to the spectrometer either by DHCP or using the FCONF program.

Depending on the type of the IP address assignment, the spectrometer DIP switches have to be positioned as follows:

	Position of the DIP switches for an IP address assignment by DHCP ☞ For information about a DHCP-based IP address assignment, see section 3.8.6.2.
	Position of the DIP switches for the assignment of a static IP address using the FCONF program ☞ For information about how to assign a static IP address to the spectrometer, see section 3.8.6.3.

How to get access to the spectrometer DIP switch

1		1. Remove the plastic cover ① which provides access to the DigiTect detector. Note: This cover is held in place magnetically.
2		2. Remove the metallic cover ②.
3		③ - Location of the DIP switch

3.8.6.2 IP address assignment by DHCP

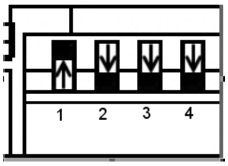
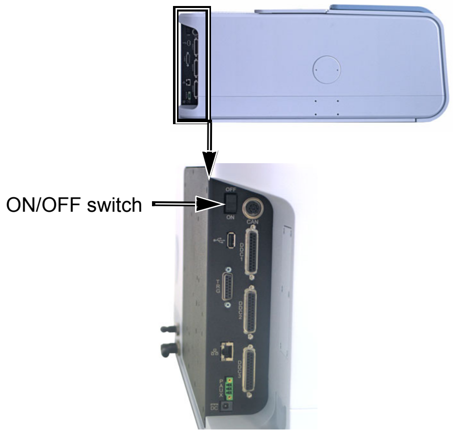
General Information

➢ A DHCP[1]-based IP address assignment requires a DHCP server integrated into the local network.

By DHCP, the following types of IP addresses can be assigned:

- **Static IP address, also called static DHCP, also known as DHCP reservation (preferred variant):** In this case, the DHCP server always assigns automatically the same IP address to spectrometer which the network administrator has "reserved" on the DHCP server for the spectrometer in advance.
- **Dynamic IP address (not recommended):** In this case, the DHCP server assigns automatically a random IP address from a pool of available IP addresses. This means, each time the spectrometer reboots most likely a different IP address is assigned to the spectrometer.

Procedure

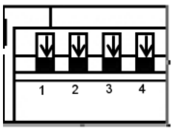
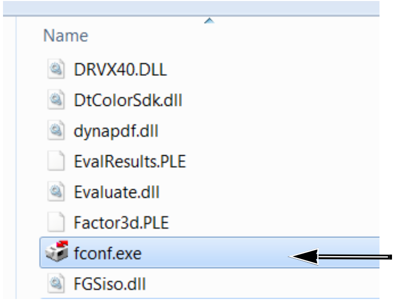
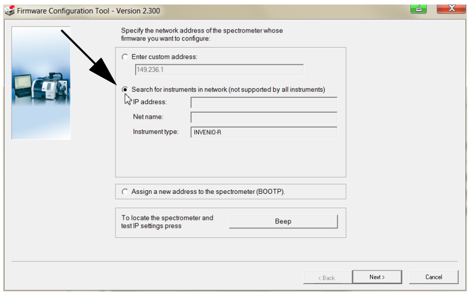
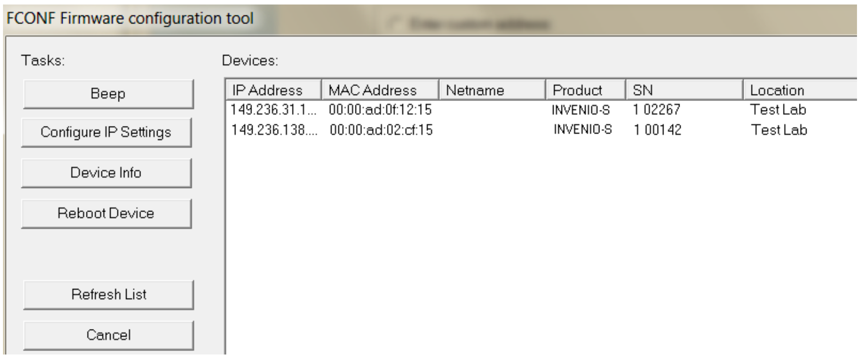
1	**Only in case of static DHCP:** On the DHCP server, the network administrator has to set up a DHCP reservation (i.e. a certain IP address) for the spectrometer in question (on the basis of the spectrometer MAC address).	
2		Check whether the first DIP switch is put up (i.e. in the ON position) and all the other DIP switches are put down (i.e. in the OFF position). If not, position them so now.
3		Restart the spectrometer by switching it off and on again.
4	➢ After the spectrometer reboot is finished, the DHCP server assigns automatically an IP address to the spectrometer.	

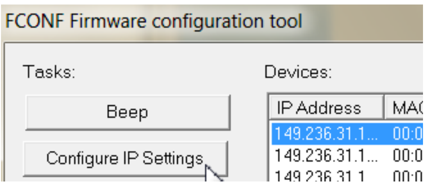
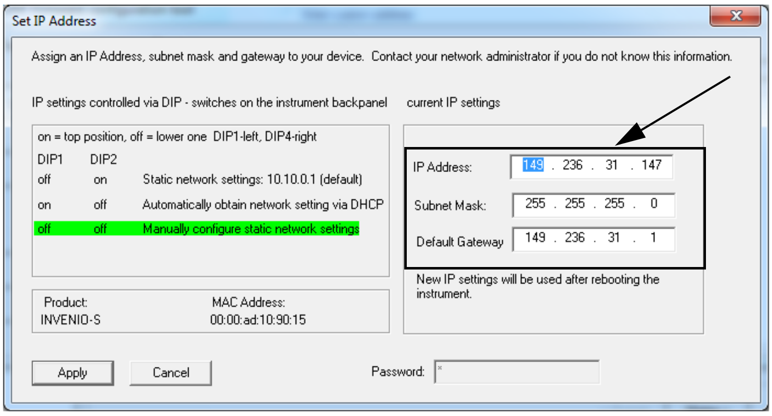
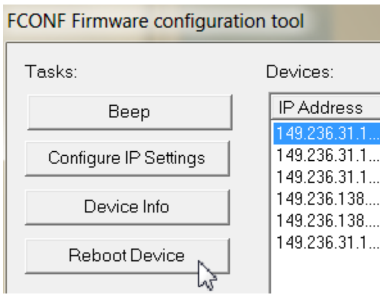
---

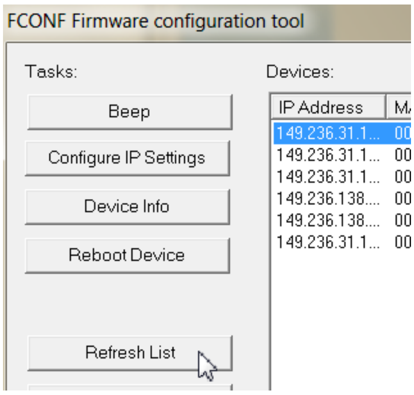
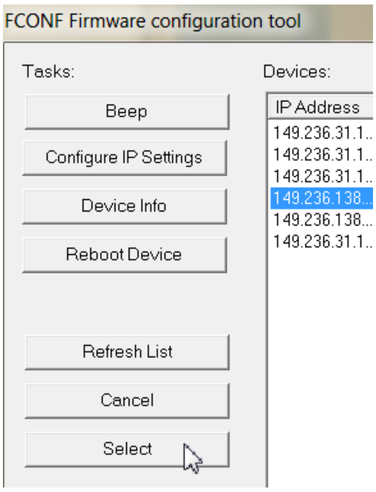
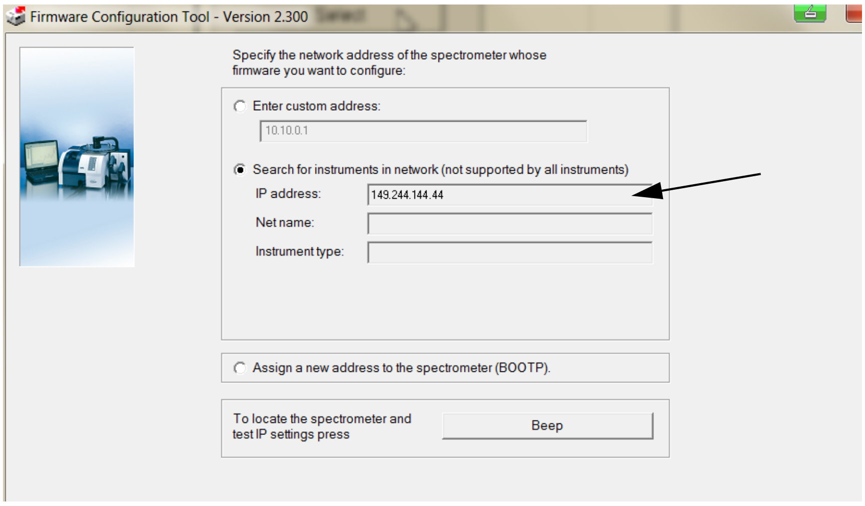
[1] DHCP (<u>D</u>ynamic <u>H</u>ost <u>C</u>onfiguration <u>P</u>rotocol) is a protocol that automatically assigns IP addresses to the devices connected in a network. If several devices (e.g. PCs, spectrometers etc.) are connected to a local network simultaneously, the DHCP server assigns a unique IP address to each device. Possible access problems are thus avoided. In principle, the external PC can also be connected to the DHCP server via WLAN. In case of a WLAN connection, the transmission rate must be high, at least 54 MBit/s.

3.8.6.3 Assigning a static IP address to the spectrometer using FCONF

The static IP address has to be defined by the network administrator.

<table>
<tr><td>1</td><td> </td><td>Check whether all DIP switches are put down (i.e. in the OFF position). If not, position them so now.</td></tr>
<tr><td>2</td><td>Name
DRVX40.DLL
DtColorSdk.dll
dynapdf.dll
EvalResults.PLE
Evaluate.dll
Factor3d.PLE
fconf.exe
FGSiso.dll</td><td>If OPUS is already installed...:
1. Browse to <i>C:\Program\Bruker\OPUS [current version]</i>.
2. Double-click the <i>fconf.exe</i> file to start the FCONF program.
If OPUS is not yet installed...:
1. Insert the OPUS installation USB stick into the USB port of the PC.
2. Browse to the <i>fconf.exe</i> file and double-click the <i>fconf.exe</i> file to start the FCONF program.</td></tr>
<tr><td>3</td><td>Firmware Configuration Tool - Version 2.300
Specify the network address of the spectrometer whose firmware you want to configure:
○ Enter custom address: 149.236.1
● Search for instruments in network (not supported by all instruments)
IP address:
Net name:
Instrument type: INVENIO-R
○ Assign a new address to the spectrometer (BOOTP).
To locate the spectrometer and test IP settings press Beep
< Back | Next > | Cancel</td><td>- Activate the <i>Search for instrument in network</i> option button.
- Click the <i>Next</i> button.</td></tr>
<tr><td>4</td><td colspan="2">- Select the spectrometer from the list box.
FCONF Firmware configuration tool
Tasks: Beep | Configure IP Settings | Device Info | Reboot Device | Refresh List | Cancel
Devices:
IP Address | MAC Address | Netname | Product | SN | Location
149.236.31.1... | 00:00:ad:0f:12:15 | | INVENIO-S | 1 02267 | Test Lab
149.236.138.... | 00:00:ad:02:cf:15 | | INVENIO-S | 1 00142 | Test Lab
i The list box contains all spectrometers connected to the network, or directly to a PC.
- Check whether the selected spectrometer is detected by the firmware. to do this, click the <i>Beep</i> button. If the spectrometer beeps once, it has been detected by the firmware.</td></tr>
</table>

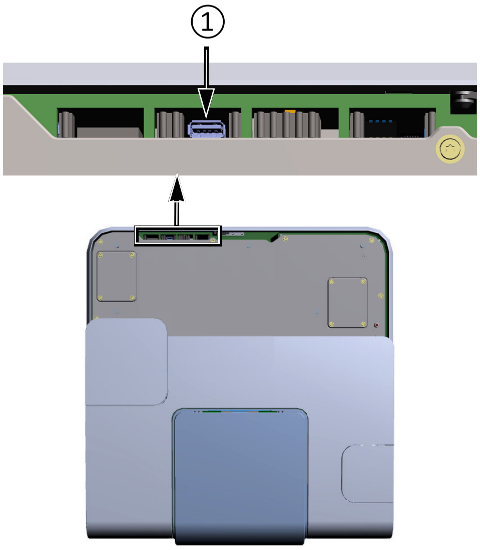
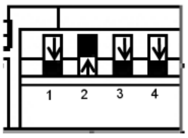
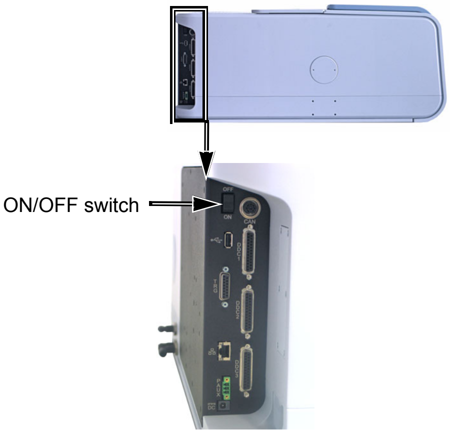
5	 149.236.31.1... 00:0 149.236.31.1... 00:0 149.236.31.1 00:0	Click the *Configure IP Settings* button.
6	- Enter the IP address, subnet mask and gateway.  Assign an IP Address, subnet mask and gateway to your device. Contact your network administrator if you do not know this information. IP settings controlled via DIP - switches on the instrument backpanel on = top position, off = lower one DIP1-left, DIP4-right DIP1 DIP2 off on Static network settings: 10.10.0.1 (default) on off Automatically obtain network setting via DHCP off off Manually configure static network settings Product: INVENIO-S MAC Address: 00:00:ad:10:90:15 current IP settings IP Address: 149 . 236 . 31 . 147 Subnet Mask: 255 . 255 . 255 . 0 Default Gateway 149 . 236 . 31 . 1 New IP settings will be used after rebooting the instrument. Password: * - Click the *Apply* button.	
7	 149.236.31.1... 149.236.31.1... 149.236.31.1... 149.236.138.... 149.236.138.... 149.236.31.1...	Click the *Reboot Device* button.
8	 Product Name: INVENIO-S MAC Address: 00:00:ad:0b:5d:15 Password: * To reboot your instrument, please press the rboot-button.	- Click the *Reboot* button. - Click the *Close* button. ➢ The spectrometer reboots. After 30 to 60 seconds the list box, which contains all spectrometers connected to the network, is displayed again.

9	 149.236.31.1... 00 149.236.31.1... 00 149.236.31.1... 00 149.236.138.... 00 149.236.138.... 00 149.236.31.1... 00	Click the *Refresh List* button to refresh and check the entries in the list box.
10	 149.236.31.1.. 149.236.31.1.. 149.236.31.1.. 149.236.138... 149.236.138... 149.236.31.1..	- Select the spectrometer IP address in the list box. - Click the *Select* button.
11	The *IP address* field must now contain the updated IP address.  Specify the network address of the spectrometer whose firmware you want to configure: ○ Enter custom address: 10.10.0.1 ● Search for instruments in network (not supported by all instruments) IP address: 149.244.144.44 Net name: Instrument type: ○ Assign a new address to the spectrometer (BOOTP). To locate the spectrometer and test IP settings press	

3.8.6.4 Reassigning the standard IP address to the spectrometer

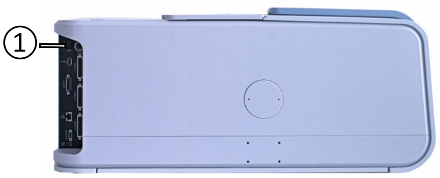
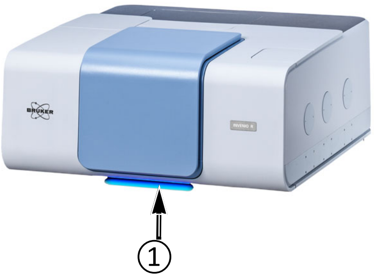
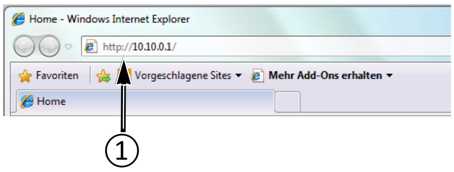
By default, the spectrometer is delivered with the factory-assigned standard IP address 10.10.0.1. This is the spectrometer IP address for the connection variants A and C, you do not need to assign a different IP address to the spectrometer.

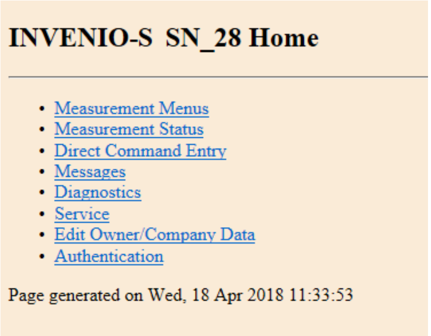
If the standard IP address has been changed for whatever reason, you can reassign the standard IP address to the spectrometer using the DIP switch. Proceed as follows:

1		① - Location of the DIP switch ☞ For information about how to get access to the DIP switch, see section 3.8.6.1.
2		Position the DIP switches as follows: • 2nd DIP switch: up (ON status) • 1st, 3rd and 4th DIP switch: down (OFF status)
3		Restart the spectrometer by switching it off and on again.
4	➢ After the spectrometer reboot is finished, the standard IP address (10.10.0.1) is assigned to the spectrometer.	

3.8.7 Checking the communication between the spectrometer and the PC

After having connected the data cable(s) and, if required, assigned different network addresses to the spectrometer and/or the PC, it is recommended to check the communication between the spectrometer and the PC. To do this, proceed as follows:

<table>
<tr>
<td>1</td>
<td> </td>
<td>Switch on the spectrometer using the ON/OFF switch ① at the spectrometer rear side.
Switch on the PC.</td>
</tr>
<tr>
<td>2</td>
<td> </td>
<td>Wait until the spectrometer and the PC have finished booting up and are ready to operate.
Note: The status LEDs ① light up bluish only for the duration initialization of the spectrometer.
➢ For detailed information about the status LEDs, see section 4.1.1.</td>
</tr>
<tr>
<td>3</td>
<td colspan="2">Start an Internet browser.
Check whether the Internet browser is not in the offline mode.
Ensure that the Internet browser does not use a proxy server, or at least not for addresses of direct access in the 10.10.x.x-range.</td>
</tr>
<tr>
<td>4</td>
<td>http://10.10.0.1/ </td>
<td>Enter the spectrometer IP address in the Internet browser entry field ① and press the ENTER key.
• If the spectrometer is connected directly to an external PC, the standard IP address is 10.10.0.1.
• In case of a DHCP-assigned IP address, you can enter instead of the IP address <i>invenio-s-SN</i> with <i>SN</i> being the serial number of the spectrometer in question. Note: You find the serial number of the spectrometer on the type label at the spectrometer rear side.
• In case the spectrometer is directly connected to a network and a static IP address has been assigned using the FCONF program, you can retrieve the IP address as described in section E.6.</td>
</tr>
</table>

5	 **INVENIO-S SN_28 Home** - Measurement Menus - Measurement Status - Direct Command Entry - Messages - Diagnostics - Service - Edit Owner/Company Data - Authentication Page generated on Wed, 18 Apr 2018 11:33:53	☞ In case of a successful communication between spectrometer and PC, the Internet Explorer now displays the home page of your spectrometer firmware.
	☞ If the communication fails the Internet browser shows a blank page. In this case, check the spectrometer IP address for correct spelling. If this action does not solve the problem, see section 7.5.6.	

3.9 Integrated panel PC - Connecting peripherals

The integrated panel PC with touch screen is an optional feature. The following peripherals can be connected to the panel PC:

- mouse
- keyboard
- external monitor
- printer

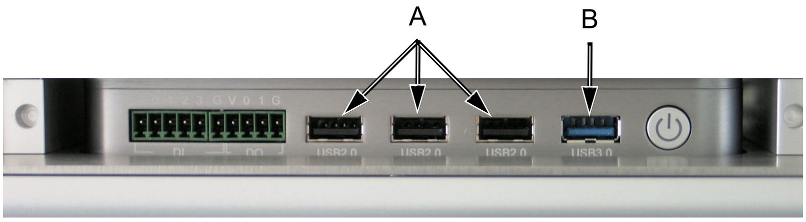


Figure 3.12: Panel PC (top side) - Connection ports

Fig. 3.12	**Connection ports for peripherals**
A	USB 2.0 port These USB ports are intended for connecting USB 2.0 compatible or WLAN- or BlueTooth-capable peripherals like mouse, keyboard or printer.
B	USB 3.0 port This USB port is intended for connecting a USB 3.0-capable storage medium, for example.

3.10 Installing the spectroscopy software OPUS

3.10.1 General information

For operating the spectrometer and performing measurements, the following OPUS software programs are available:

OPUS/IR	This software program is installed on a PC data station (e.g. PC, laptop etc.). ☞ For detailed information about OPUS/IR, refer to the OPUS Reference Manual.
OPUS/TOUCH	This software program is installed on the integrated panel PC. ☞ For detailed information about OPUS/TOUCH, refer to the OPUS/TOUCH Manual.

In case the PC has been obtained from Bruker, the PC is delivered with the OPUS/IR software being already factory-installed. In case of an INVENIO spectrometer with an integrated panel PC, the analysis system is delivered with the OPUS/TOUCH software being already factory-installed on the panel PC. In all other cases, the OPUS software needs to be installed by the operator.

3.10.2 Installing the OPUS/IR software

The OPUS/IR software is delivered on an USB stick.

Before starting the OPUS/IR installation...:

- the user must have administrator rights in Windows
- an Internet explorer must be installed on the external PC
- the external PC must be connected to the spectrometer (See section 3.8.)

To install OPUS/IR, proceed as follows:

1. Insert the OPUS installation USB stick into the USB port of the PC.
   ➢ ***Note:*** *If the installation starts automatically after the USB stick has been inserted, interrupt the installation procedure.*
2. Right-click the *SETUP.EXE* file.
3. In the pop-up menu, select the *Run as Administrator* option.

---

i When using Windows 10 or higher, it is not sufficient to be logged into the operating system as a user with administrator rights. In this case, you need to perform the installation explicitly as administrator, and start the installation manually.

---

4. Confirm the message that pops up to continue with the installation.
5. The installation program will guide you step by step through the OPUS installation procedure. Follow the on-screen instructions.
6. After the installation is finished, remove the USB stick from the USB port of the PC.

   ➢ *As soon as the installation is finished, the OPUS icon is displayed on the Windows Start menu.*

☞ For a short introduction into the OPUS software, consult the OPUS Introduction Manual. You find this manual (as PDF) on the OPUS USB stick.

3.11 Windows administrator account

Particular types of settings require administrator user rights. In case of the spectrometer configuration with panel PC and the spectroscopy software OPUS/TOUCH, you can use the Windows administrator account[1] when administrator user rights are required.

ℹ It is recommended to install an additional external keyboard to the USB 2.0 port, which is located on the top side of the touch screen. Details on the ports are described in section 3.9. If installed, you can switch between the on-screen and the external keyboard.

3.11.1 Switching to Windows administrator account from OPUS/TOUCH

1. In OPUS/TOUCH, press the *Ctrl+ALT+DEL* keys on the external keyboard.
2. In the view that opens, tap **Switch user**.
3. Select the **Admin** user account.
4. Enter the password[2] and tap the **ENTER** key to confirm it.

   ➢ *The Windows desktop view is shown.*

3.11.2 Switching to OPUS/TOUCH from the Windows administrator account

Variant 1:

1. In the Windows administrator account, press the *Ctrl+Alt+Del* keys on the external keyboard.
2. Tap **Switch user**.
3. In the view that opens, tap the **TOUCH User** account.
4. Tap **Sign in**.

   ➢ *In OPUS/TOUCH, the view is shown which you had last open.*

---

[1] Windows 10 or higher is required.

[2] By default, the password is *Seahorse*.

Variant 2:

1. In the Windows administrator account, open the *Start* menu.
2. Tap the 👤 icon.
3. Tap the **TOUCH User signed in** option.
4. In the view that opens, tap **Sign in**.
   ➢ *In OPUS/TOUCH, the view is shown which you had last open.*

3.11.3 After a restart of the panel PC

After a restart of the panel PC, the user account is always displayed which you have last worked with, i.e. *Admin* or *TOUCH User*.

4 Overview

This chapter provides an overview of all user-relevant external and internal spectrometer components

4.1 Outside view

Figure 4.1: General spectrometer overview (outside view)

Fig. 4.1	Description
A	Cover providing access to the DigiTect-type detector
B	Cover providing access to the large-sized sample compartment
C	Spectrometer status indicator (LED strip below the sample compartment)
D	IR beam outlet ports
E	Cover providing access to the small-sized sample compartment
F	Panel PC with touch screen (optional feature)

4.1.1 Spectrometer status indicator

Figure 4.2: Location of the spectrometer status indicator

Below the large sample compartment, there is a LED strip which indicates the current spectrometer status. The color of the LEDs give a general indication of the operating status of the spectrometer.

LEDs light up bluish.	The spectrometer is initializing. Note: The LEDs light up bluish only for the duration of spectrometer initialization.
LEDs light up blue.	Instrument is OK and ready for measurement. This is the case when: • all optical components (e.g. source, laser) achieve their performance specification and • the OVP tests (OQ and PQ) of the currently selected measurement channel have passed and are still valid.
LEDs light up yellow.	A yellow instrument status indicates a warning. This is the case when: • the end of the specified lifetime of the source and/or laser is nearly reached or • the validity period of an OVP test (OQ and/or PQ) of the currently selected measurement channel is expired or • an OVP test (OQ and/or PQ) of the currently selected measurement channel has failed or • the water vapor concentration inside the spectrometer is too high, i.e. it exceeds the factory-set limit value. Note: In case of a yellow instrument status LED, measuring is still possible, but the reliability of the measurement results is not ensured. For this reason, it is highly recommended to diagnose the cause of the warning and to eliminate it. **Important note:** In case you work in a validated environment, you have to diagnose the cause of the warning and to eliminate it before continuing with the measurements. Otherwise, 21CFR part 11-compliant measurement results are not ensured.

LEDs light up red.	A red instrument status LED indicates an error. For example, this is the case when: • an optical component (e.g. NIR source, laser) fails or does not achieve its performance specification Note: In case of a red instrument status LED, measuring is not possible. Before you can proceed with the measurement, you have to diagnose and eliminate the cause of the fault. ☞ For a systematic fault diagnosis see section 7.3.

4.1.2 Sample compartments

The following sample compartments are available:

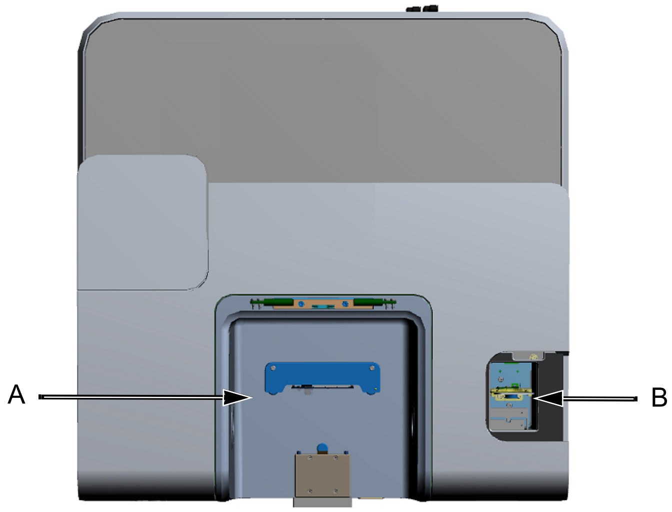
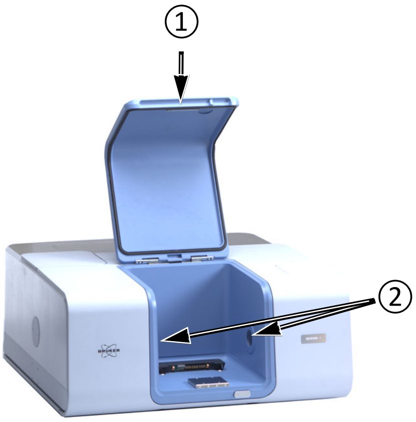
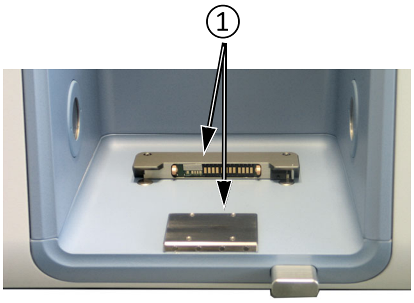


Figure 4.3: Location of the sample compartments

Fig. 4.3	Description
A	**Standard:** large-sized sample compartment with QuickLock mechanism for positioning QuickLock-type accessories in the sample compartment ☞ For information about how to place a QuickLock-type accessory in the sample compartment, see section 5.4.
B	**Option:** small-sized sample compartment with slide-bracket for slot-in accessories Note: Depending on the accessory to be used, the slide bracket can be relocated between two positions. ☞ For information about how to relocate the slide bracket see section 4.1.2.2.

4.1.2.1 Sample compartment with QuickLock

	Open the sample compartment by turning the sample compartment cover ① upwards. The circular openings ② on either side of the sample compartment are closed either by windows or automatic shutters. ☞ For information about the available window materials, see section 4.5.5. ☞ For information about how to exchange a window, see section 6.4. ☞ For information about the automatic shutters, see section 5.4.5 and section 5.8.
 	To install bulky accessories inside the sample compartment you can remove the sample compartment cover by pressing the release button ... ...while taking off the cover.

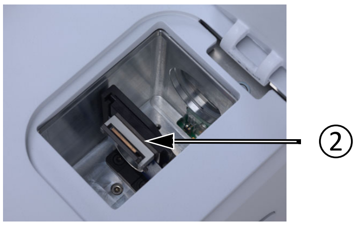
	The sample compartment is equipped with a QuickLock locking mechanism ① which allows for an exact and reproducible positioning of the accessory in the sample compartment, provided that the accessory is mounted on a QuickLock base plate. ☞ For information about how to place a QuickLock-type accessory in the sample compartment, see section 5.4.

i Bruker offers a large variety of QuickLock-type measurement accessories which are designed for dedicated R&D applications.

4.1.2.2 Small-sized sample compartment (option)

The small-sized sample compartment is an optional feature. It allows for MIR measurements without the need for removing an accessory setup possibly installed in the main sample compartment.

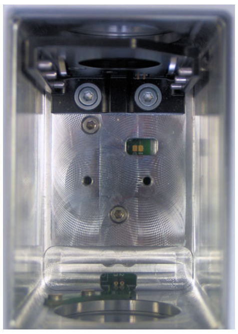
Open the sample compartment by turning the sample compartment cover ① upwards.



This sample compartment is equipped with a slide bracket ② to slide in the available accessories.

A variety of sample accessories is available: Pellet holder, magnetic holder for films, clamp holders for different kind of flat samples, gas and liquid cells etc.

Depending on the accessory to be used, the slide bracket can be relocated between the following two positions:



Slide bracket in the **rear position** when using the following accessories: gas cell and reflection unit

Slide bracket in the **center position** when using the following accessories: pellet holder, foil holder and liquid cell

To relocate the slide bracket, proceed as follows: Loosen the two TORX screws at the base plate of the slide bracket using the supplied TORX (TX 20) screwdriver. Locate the slide bracket to the other position. Mount the slide bracket by tightening the two TORX screws at the base plate of the slide bracket.

The following figure illustrates how to use the available accessories.

Pellet holder 	**Foil holder** 
Reflection unit 1. Sliding in the reflection unit. 	2. Placing the sample on the reflection unit. 
Gas cell 1. Sliding in the gas cell holder. 	2. Gas cell correctly placed on the holder. 
Liquid cell 1. Applying the sample solution on the cell. 	2. Assembling the liquid cell. 
3. Inserting the liquid cell in the holder. 	4. Sliding in the liquid cell holder. 

Figure 4.4: Small-sized sample compartment - Available sample accessories in use

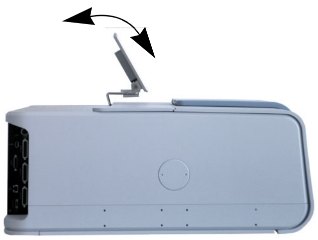
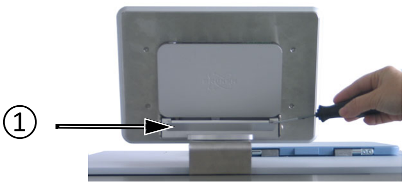
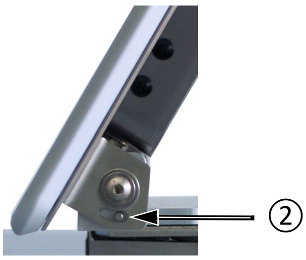
☞ For detailed information about the relevant sample preparation techniques (e.g. pressing a KBr pellet etc.), see appendix F.

4.2 Touch panel PC

Optionally, INVENIO S is equipped with an integrated touch panel PC for operating the spectrometer with the software package OPUS/TOUCH.

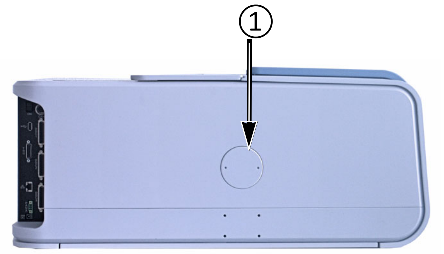
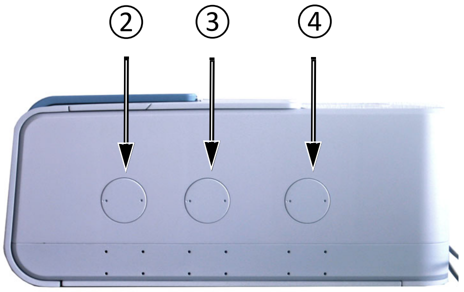
☞ For detailed information about the OPUS/TOUCH software, refer to the OPUS/TOUCH Manual.

According to the user’s needs, the touch panel can be...:

	... tilted up- and downwards to some degree (± 15°)
	... turned to the left and right to some degree (0° to 25°)
	... slided between the right position and the position near to the center.
  	For transport purposes, the touch panel PC can be folded back. Note: To do this, first remove the magnetically fixed slat ① using a suitable object (e.g. a small slot screwdriver. While pressing in the pin ② fold back the touch panel PC.

4.3 IR beam ports

The spectrometer has three IR beam outlet ports which allow the coupling / connection of accessories (e.g. FTIR microscope, HTS-XT module) to the spectrometer. (See section 2.6.)

	**Left spectrometer side** ① - Outlet port for a parallel IR-beam (e.g. for connecting the FTIR microscope HYPERION or an external detector chamber)
	**Right spectrometer side** ② - Outlet port for a parallel IR-beam (Note: This port cannot be used if the spectrometer has an optional, small-sized sample compartment.) ③ - Outlet port for a parallel IR-beam (e.g. for connecting the FTIR microscope HYPERION) ④ - This port is not used in case of INVENIO S.

i External accessories (e.g. FTIR microscope HYPERION) are coupled to the spectrometer by a Bruker service technician only.

	If there is not any accessory coupled to the spectrometer, the ports are closed by a blind flange. If an accessory is coupled to the spectrometer, the blind flange is substituted for a window. (Available windows are listed in section B.2.) Both the blind flange and the window are held by magnets. For removing or installing the blind flange or window from the IR beam outlet or inlet port use the special tool which is included in the delivery scope.

4.4 Ports and connectors at the spectrometer rear side

This section provides an overview of the ports and connectors at the spectrometer rear side.

General overview

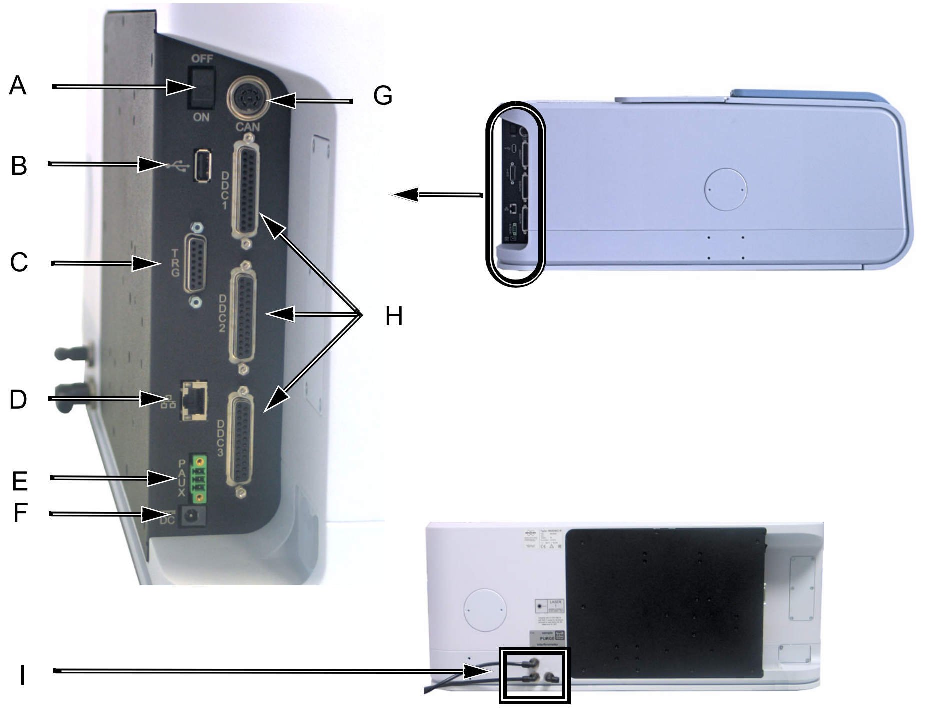


Figure 4.5: Spectrometer rear side - General overview

Fig. 4.5	Ports, connectors and buttons
A	ON/OFF switch for switching on / off the spectrometer ☞ For information about the switch-on / switch off- procedure, see section 5.2 and 5.3.
B	USB port for connecting USB-capable accessories
C	TRG (15-pin D-SUB female connector) This connector is intended for the connection of a triggering device. It is used in conjunction with the Step Scan option or Rapid Scan option for rapid scan or step scan and time-resolved measurements. (The abbreviation TRG stands for "Trigger".) ☞ For detailed information refer to the Step Scan Manual or Rapid Scan Manual.

Fig. 4.5	**Ports, connectors and buttons**
D	Ethernet port This port is used to connect the spectrometer to a PC or to a network. The is designed for RJ-45 plugs and complies with the Ethernet standard 10/100/1000Base-T. ☞ For detailed information, see section 3.8.
E	PAUX port for power supply of externally connected accessories
F	Low-voltage socket The low-voltage socket is used to connect the low-voltage cable of the external power supply unit to spectrometer. ☞ For information about how to connect the spectrometer to the mains power supply, see section 3.6.
G	CAN bus port (for connecting motorized accessories) The CAN bus connector is primarily used to connect external automated units (e.g. sample changer, moving mirror unit, etc.) to the spectrometer. The CAN bus also provides power to these units. Thus, most external units can be operated without connecting them to the power supply. Furthermore, the CAN bus can be used as a communication link to control these external units via the spectrometer. (The abbreviation CAN stands for Controller Area Network.)
H	DDC1 to DDC3 ports The ports DDC 1 to DDC3 are versatile ports to connect external optical modules and detectors. These ports include a complete CAN bus, transmits all required remote trigger signals and establishes a complete connection to DDC (Digital Detector Connection) compatible detectors.
I	2x purge gas inlets (for purging the sample compartment and the optical bench) and 1x purge gas outlet (in case the optical bench is purged) ☞ Note: For information about how to connect the spectrometer to a purge gas supply line, see section 3.7.

4.5 Inside view

4.5.1 Overview

Figure 4.6 shows the location of the most important internal spectrometer components.

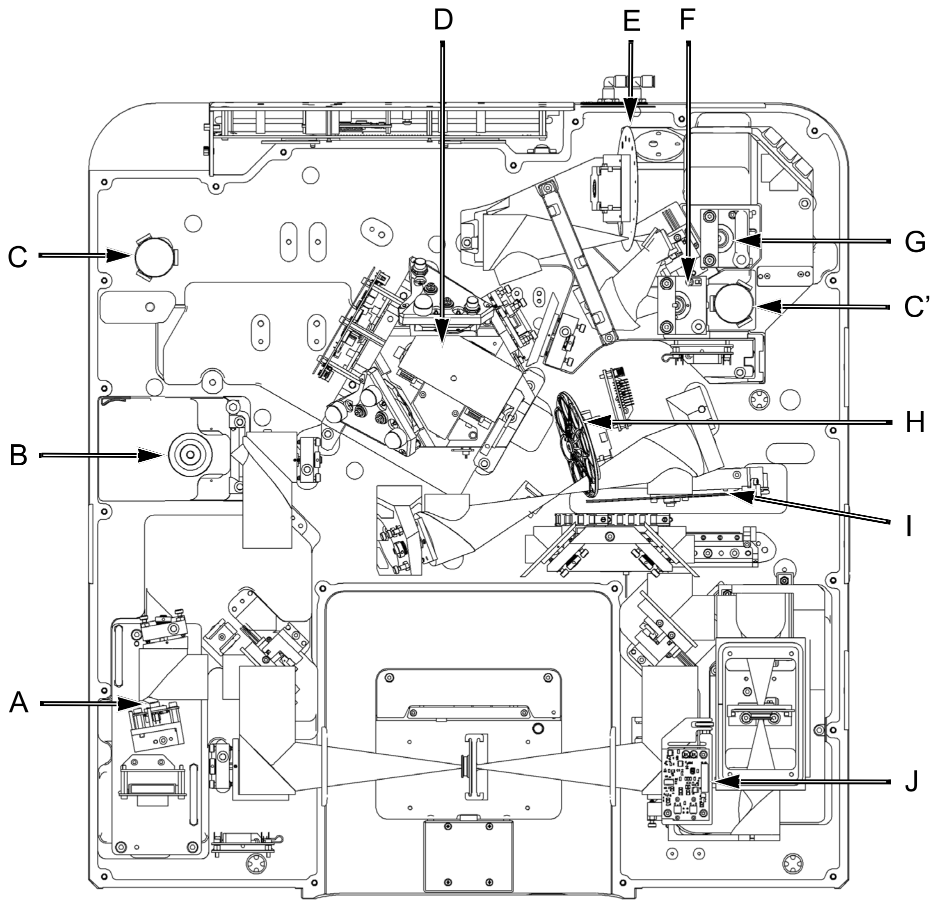


Figure 4.6: Internal spectrometer components

Fig. 4.6	Internal spectrometer component
A	Standard detector (DLaTGS with KBr window) Note: In case of INVENIO S with CsI optics: DLaTGS with CsI window
B	Detector (DigiTect-type) Note: At this position, an optional MCT detector can be installed.
C & C'	Desiccant cartridges
D	RockSolid interferometer block (including laser diode and factory-installed beamsplitter)

Fig. 4.6	Internal spectrometer component
E	Aperture wheel
F	NIR source (optional)
G	MIR source (standard)
H	Filter wheel (IVU - Internal Validation Unit) Note: This wheel has eight filter positions, six of them are factory-equipped with filters for validation purposes. Two positions are vacant. They can be equipped with additional filters.
I	Attenuator wheel (It is a perforated grid wheel with different grid sizes for an additional attenuation of the IR beam.) Note: The attenuator wheel is an optional feature.
J	Detector unit of the small-sized sample compartment (room temperature DTGS)

4.5.2 Source

Standard source

The spectrometer is equipped a MIR source which is installed inside the spectrometer (G in fig. 4.6). The MIR source is a globar (i.e. an U-shaped silicon carbide piece) which emits mid-infrared light. It is air-cooled, i.e. it does not require special cooling. With this source, spectroscopic measurements in the mid-infrared region can be performed.

Optional source

In case of the optional spectrometer variant with the broadband KBr beamsplitter, a NIR source is installed inside the spectrometer in addition to the MIR source.

Type of source	Mode of cooling	Installation location
NIR source (tungsten halogen lamp)	air-cooled	installed in the spectrometer

With the optional NIR source, spectroscopic measurements in the near-infrared region can be performed.

➢ **Important note:** The combination of source, beamsplitter and detector defines the IR measurement range. So, for spectroscopic measurements in the near-infrared region, make sure that a NIR-detector is installed.

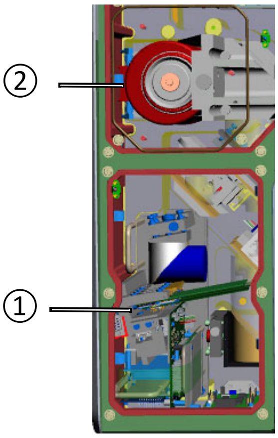
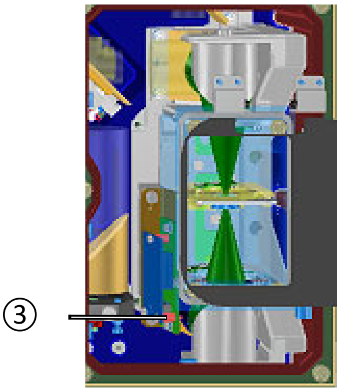
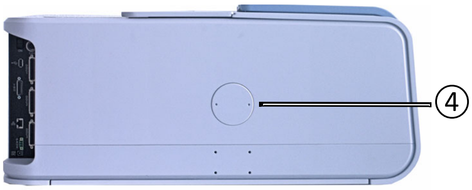
☞ The available optional NIR detectors are listed in section 4.5.3.

☞ For information about how to install a detector, see section 5.9.

4.5.3 Detector

General information

All available detectors are equipped with an integrated preamplifier and an A/D converter that converts the analog signal from the detector directly into a digital signal. This so called DigiTect technology allows for an interference-free signal transmission and ensure a high signal-to-noise-ratio.

	The spectrometer can be equipped with the following detectors: ① - Standard detector (RT DTGS detector for MIR measurements, stationary) ② - DigiTect-type detector (e.g MCT detector, DLaTGS detector) Note: The detectors installed in this position are mounted on a dovetail slide which allows an easy exchange. See also section 5.9. ➢ These detectors are available for measurements performed with the large-sized sample compartment.
	For measurements performed with the small-sized sample compartment, the following detector is available: ③ - DTGS detector (room temperature)
	At the IR beam outlet port ④ at the left spectrometer side, an optional bolometer detector can be connected.
The detector which is used for the measurement is selected by the user in OPUS.	

Standard detector (for measurements with the large-sized sample compartment)

The standard detector is installed stationary inside the spectrometer, i.e. this detector can not be exchanged.

For all spectrometer variants, except for the optional variant with CsI optics, the following detector is the standard one:

Detector	Spectral range (cm^{-1})	Sensitivity	Operating temperature / cooling method
DLaTGS with KBr window	12,000 - 350	$D^*>2x10^8 cm\ Hz^{1/2}W^{-1}$	Room temperature, no additional cooling required

For the optional spectrometer variant with CsI optics, the following detector is the standard one:

Detector	Spectral range (cm^{-1})	Sensitivity	Operating temperature / cooling method
DLaTGS with CsI window	12,000 - 130	$D^*>2x10^8 cm\ Hz^{1/2}W^{-1}$	Room temperature, no additional cooling required

Detector (for measurements with the small-sized sample compartment)

For measurements with the small-sized sample compartment, only one detector is available:

Detector	Spectral range (cm^{-1})	Sensitivity	Operating temperature / cooling method
Mid-Infrared			
DLaTGS with KBr window	12,000 - 350	$D^*>4x10^8 cm\ Hz^{1/2}W^{-1}$	room temperature (Note: Temperature stabilization is an optional feature.)

DigiTect detectors (for measurements with the large-sized sample compartment)

For installing a DigiTect detector, there is an additional detector position which is an optional feature. The DigiTect-type detectors are mounted on a dovetail slide which allows an easy exchange. A re-alignment is not necessary.

Optional MIR detectors

The available optional MIR detectors differ from each other mainly in terms of detection sensitivity. The following optional MIR detectors are available:

Detector	Spectral range (cm^{-1})	Sensitivity	Operating temperature / cooling method
MCT narrow band, with BaF_2 window **HARMFUL!**	12,000 - 850	D*:>$4x10^{10}$cm $Hz^{1/2}$ W^{-1}	Liquid N_2 cooled
MCT mid band, with ZnSe window **TOXIC!**	12,000 - 600	D*:>$2x10^{10}$cm $Hz^{1/2}$ W^{-1}	Liquid N_2 cooled
MCT broad band, with KRS-5 window **TOXIC!**	12,000 - 420	D*:>$5x10^{9}$cm $Hz^{1/2}$$W^{-1}$	Liquid N_2 cooled
Photovoltaic MCT, with BaF_2 window **HARMFUL!**	12,000 - 850	D*:>$3x10^{10}$cm $Hz^{1/2}$ W^{-1}	Liquid N_2 cooled
MCT with ZnSe window (AR coated, FOV 60°)	5,000 - 700	D*:>$4x10^{10}$cm $Hz^{1/2}$ W^{-1}	with cryo-cooler

i Only for the spectrometer variant with CsI optics, the usage of the above listed MIR detectors is not recommended. In this case, use only the installed DLaTGS detector with CsI window.

Optional NIR detectors

Only for the optional spectrometer variant with the broadband KBr beamsplitter, the following NIR detectors are available in addition:

Detector	Spectral range (cm^{-1})	Sensitivity	Operating temperature / cooling method
InSb	10,000 - 1,850	D*:>$1.5x10^{11}$cm $Hz^{1/2}$ W^{-1}	Liquid N_2 cooled
InAs detector	12,800 - 3,300	NEP<$1x10^{-12}$ W $Hz^{-1/2}$	thermo-electrically cooled

Safety notes

Some detectors are equipped with windows of which the material is harmful or toxic. During normal spectrometer operation, these materials do not pose any health hazard. However, should such a detector window break because of mechanical impact, be extremely careful.

⚠ WARNING

Health hazard because of improper handling of broken harmful or toxic detector window material

Non-observance of the following safety instructions could result in death or serious injury.

➢ Avoid generating dust of broken detector window material. This material is harmful or toxic if swallowed or inhaled.

➢ Also avoid skin and eye contact.

➢ Dispose the harmful or toxic material according to the laboratory regulations and the national regulations.

➢ Observe also the safety and handling instructions given in the safety data sheet for the material in question.

☞ For detailed information about how to exchange a DigiTect detector, see section 5.9.

4.5.4 Beamsplitter

The beamsplitter is an integral part of the interferometer. This means the beamsplitter is factory-installed and cannot be replaced by the user.

Depending on the spectrometer variant, there are the following beamsplitters:

Spectrometer variant	Beamsplitter material	Spectral range (cm^{-1}) of the beamsplitter
variant with standard KBr beamsplitter (standard variant)	KBr	8,000 - 350
variant with broadband KBr beamsplitter (optional variant)	KBr	10,000 - 400
variant with CsI optics (optional variant)	CsI **HARMFUL!**	5,000 - 200
high humidity variant with ZnSe optics (optional variant)	ZnSe **TOXIC!**	5,000 - 500

Safety notes

There are beamsplitters of which the optical material is harmful or toxic. During normal operation, it does not pose any health risk. However, if it should break caused by mechanical impact, be extremely careful and observe the following safety instructions:

⚠ WARNING

Health hazard because of improper handling of broken harmful or toxic beamsplitter material

Non-observance of the following safety instructions could result in serious injury.

- ➢ Avoid generating dust of broken beamsplitter material. The material is toxic if swallowed or inhaled.
- ➢ Avoid any skin and eye contact.
- ➢ Dispose the toxic material according to the laboratory regulations and the national regulations.
- ➢ Observe also the safety and handling instructions given in the safety data sheet for the material in question.

4.5.5 Sample compartment windows

General information

There is a circular opening on either side of the large-sized sample compartment. (See fig. 4.7.) By default, these openings are closed by IR-transparent windows which are fixed magnetically to the sample compartment walls. The windows are electronically coded, i.e. they are recognized automatically by the instrument firmware.

Note: Instead of the sample compartment windows, optionally the spectrometer can be equipped with automatic shutters. These shutters open automatically as soon as the user closes the sample compartment. And they close automatically as soon as the user opens the sample compartment.

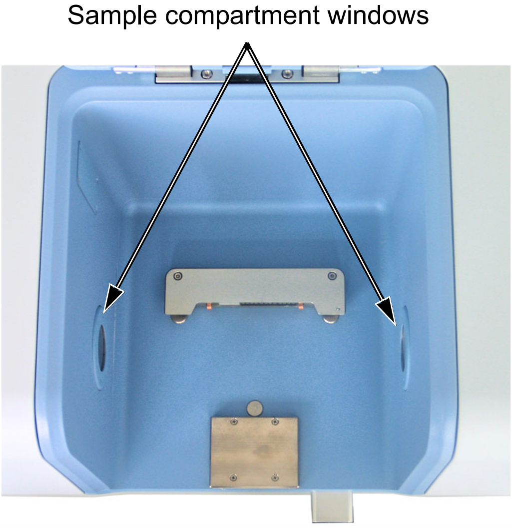


Figure 4.7: Location of the sample compartment windows

Overview of the available window materials

The following table lists the available window materials including their transmission range, refraction index and chemical properties.

Material	**Transmission range (cm^{-1})***	**Refraction index n (at 2000 cm^{-1})**	**Chemical properties**
Potassium Bromide, KBr	33,000 - 280	1.54	Soluble in water, alcohol, and glycerine; hygroscopic
Cesium Iodide, CsI **HARMFUL!**	33,000 - 180	1.74	Soluble in water and alcohol; hygroscopic
Zinc Selenide, ZnSe **TOXIC!**	20,000 - 500	2.43	Soluble in strong acids and in HNO_3, insoluble in water

50% value at a window thickness of 4mm

Safety notes

Some sample compartment windows are of a material which is harmful or toxic. During normal spectrometer operation, these materials do not pose any health hazard. However, should such a window break because of mechanical impact, be extremely careful and observe the following safety instructions.

⚠ WARNING

Health hazard because of improper handling of broken harmful or toxic window material

Non-observance of the following safety instructions could result in death or serious injury.

➢ Avoid generating dust of broken window material. This material is harmful or toxic if swallowed or inhaled.

➢ Also avoid skin and eye contact.

➢ Dispose the harmful or toxic material according to the laboratory regulations and the national regulations.

➢ Observe also the safety and handling instructions given in the safety data sheet for the material in question.

☞ For information about how to exchange a sample compartment window, see section 6.4.

4.5.6 Laser

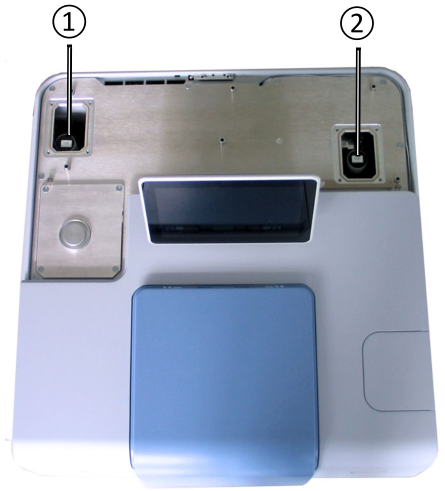
The interferometer is equipped with a semiconductor VCSEL[1] laser diode. This laser emits invisible light with a wavelength of 850 nm. The rated power output is 2 mW.

The laser controls the position of the moving interferometer mirror (also called "scanner") and is used to determine the data sampling positions. The monochromatic beam produced by the laser is modulated by the interferometer to generate a sinusoidal signal.

4.5.7 Interferometer

The spectrometer is equipped with a high stability interferometer with ROCKSOLID permanent alignment. The ROCKSOLID interferometer incorporates dual retroreflecting cube corner mirrors in pendulum arrangement. The high throughput design ensures the highest possible signal-to-noise ratio.

4.5.8 Desiccant cartridge



The spectrometer is equipped with two desiccant cartridges: ① and ②. Both desiccant cartridges are situated in the optical bench compartment.

The main purpose of the desiccant cartridges is to keep the water vapor concentration inside the spectrometer low in order to prevent the hygroscopic spectrometer components (e.g. beamsplitter, sample compartment windows) from deteriorating. The desiccant (molecular sieve) binds the air moisture inside the spectrometer.

An additional aspect for the usage of a desiccant is that water vapor in the ambient air may lead to unwanted absorptions that manifest in the spectrum. In the worst case, H_2O absorptions mask the spectral features of the sample in the spectrum. Therefore, it is necessary to reduce the water vapor content in the air inside the spectrometer.

☞ For information about how to replace and regenerate a desiccant cartridge refer to section 6.2.

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[1] VCSEL - vertical-cavity surface-emitting laser

4.6 Optical beam path

The actual beam path is determined by:

- the used source
- the used sample compartment and
- the used detector

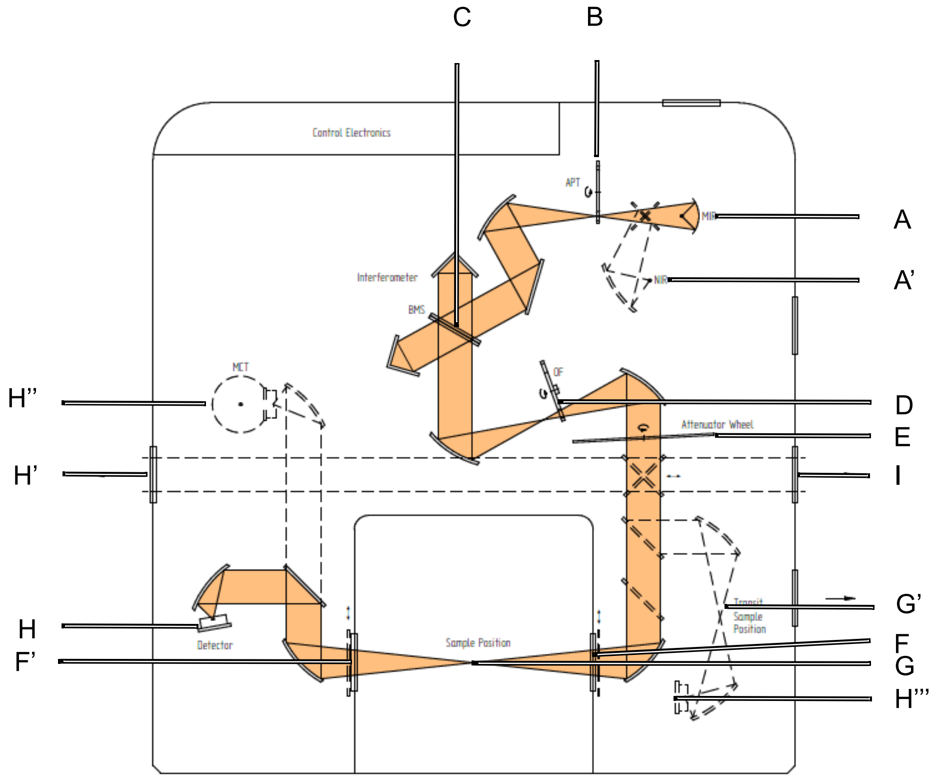


Figure 4.8: INVENIO S - Optical beam path

Fig. 4.8	Explanation
A	MIR source
A'	NIR source
B	Aperture wheel Note: The aperture wheel has 12 default wheel positions with aperture diameters ranging from 0.25 mm to 8 mm.
C	Interferometer block with integrated beamsplitter
D	Optical filter wheel (IVU - Internal Validation Unit), filter diameter: 25 mm
E	Attenuation wheel (optional component)
F	Sample compartment window (IR beam entrance into the large-sized sample compartment)

Fig. 4.8	Explanation
F’	Sample compartment window (IR beam exit of the large-sized sample compartment)
G	Sample position in the large-sized sample compartment
G’	Sample position in the small-sized sample compartment
H	Standard detector (room temperature DTGS detector), in case the large-sized sample compartment is used
H’	IR beam outlet for an externally installed detector (e.g. bolometer)
H’’	optional detector (DigiTect-type), MCT and DLaTGS, in case the large-sized sample compartment is used
H’’’	Detector (DTGS room temperature) in case the small-sized sample compartment is used
I	IR beam outlet for connecting an external accessory (e.g. Hyperion microscope)

4.7 Integrated ATR unit

4.7.1 ATR unit with exchangeable crystal plate & heatable ATR unit with Diamond crystal

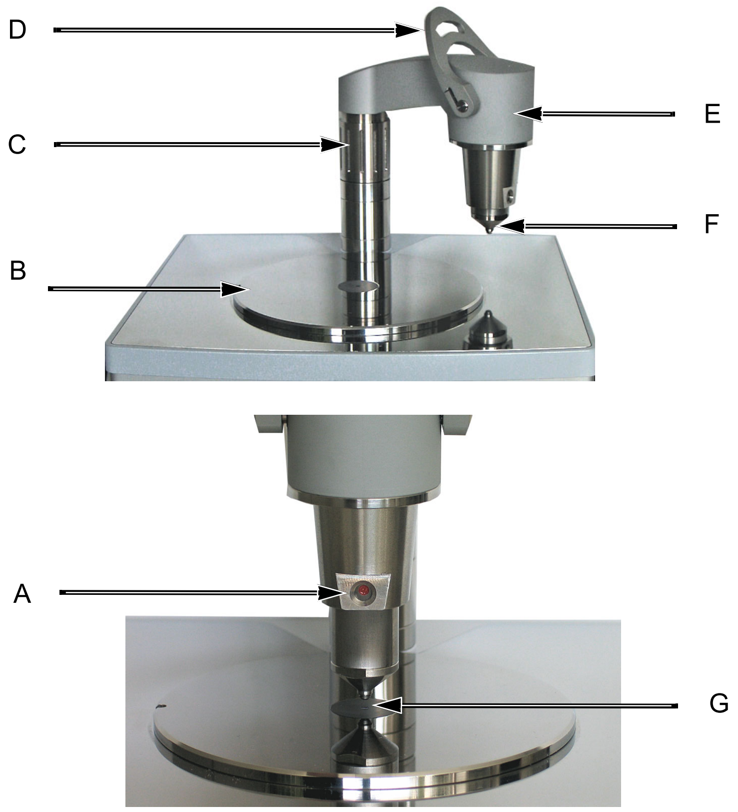


Figure 4.9: ATR Unit (upper figure: front view, lower figure: detail view)

Fig. 4.9	Operating elements / Components
A	Indication of the optimal contact pressure (Note: When the red spot is in the center of the hole, the contact pressure is OK.)
B	Crystal plate (stainless steel plate with integrated ATR crystal)
C	Knob for adjusting the height of the complete pressure application device
D	Lever for moving the anvil up and down
E	Pressure application device (pivotable to the left and to the right) Note: The purpose of this device is to apply pressure on the sample to ensure that the sample is in intimate contact with the ATR crystal
F	Anvil
G	Diamond ATR crystal (dimensions of the diamond: 2 x 2mm)

4.7.2 ATR unit with Diamond crystal, high-pressure variant

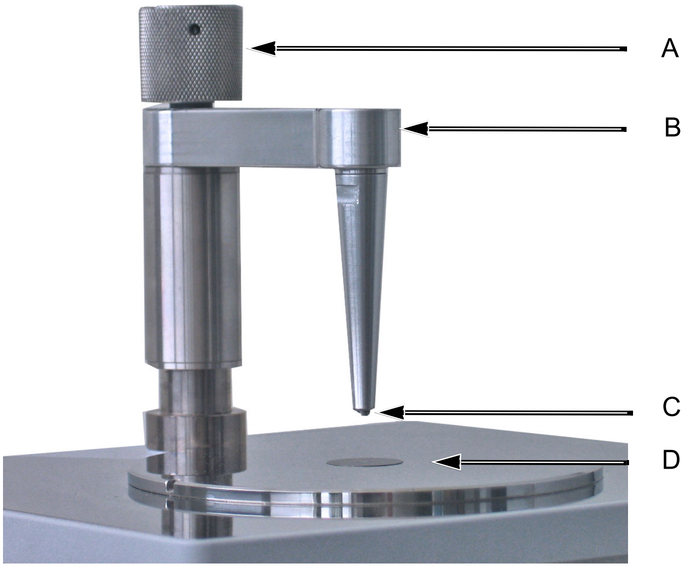


Figure 4.10: ATR unit - high-pressure variant

Fig. 4.10	Operating elements / Components
A	Knob to press and release the anvil
B	Pressure arm
C	Anvil The following anvil tip types are available: • Standard anvil tip for measuring powder, foils, work pieces etc. • Special anvil tip for measuring granular material
D	Crystal plate with integrated ATR crystal (diamond)

5 Operation

5.1 General information

The spectrometer is completely computer-controlled, i.e. operating the spectrometer (e.g. selecting the correct spectrometer component) and performing a spectroscopic measurement are done using the spectroscopic software program OPUS.

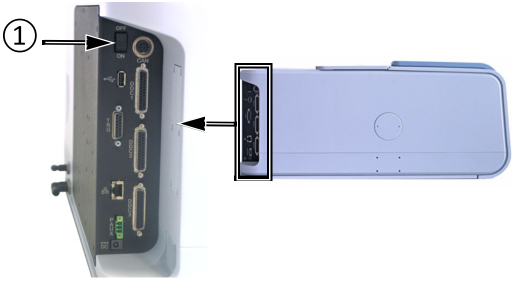
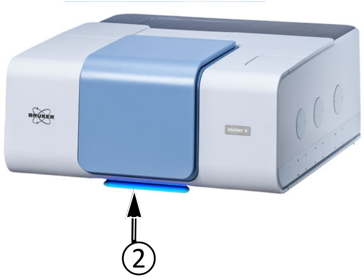
This manual is restricted mainly to the spectrometer-related aspects that are relevant to operating the spectrometer:

- switching the spectrometer on / off
- installing a QuickLock-type accessory in the sample compartment
- chronological sequence of the individual operating steps during a measurement (general measurement procedure)
- purging the spectrometer
- installing / exchanging a DigiTect-type detector (for the purpose of changing the spectral range)
- checking the signal (after the exchange of an optical component)
- cooling a detector (e.g. MCT detector) with liquid nitrogen
- measurements with the integrated ATR unit (option)

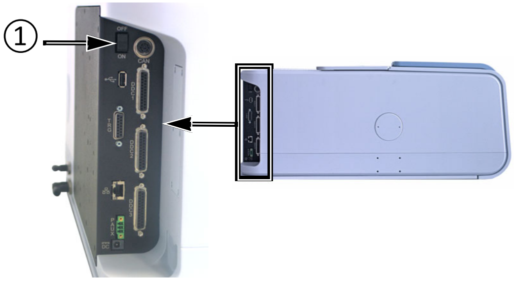
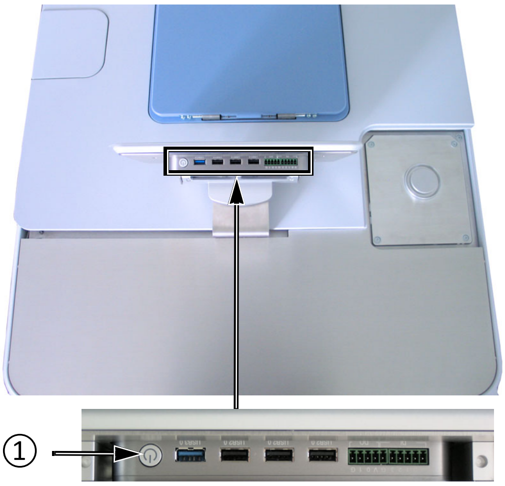
Specifying the measurement parameters and starting a measurement and evaluating the measurement results as well as defining and starting a spectrometer validation test (OQ and PQ) are done exclusively using the spectroscopic software program OPUS.

☞ For detailed information about these topics refer to the OPUS Reference Manual. For information about the measurement parameters, see also appendix C.

5.2 Switching on the spectrometer system

1		Switch on the spectrometer using the ON/OFF switch ① at the spectrometer rear side.
		Now the spectrometer starts to initialize. During the spectrometer initialization, the spectrometer status indicator ② (LED strip below the sample compartment) lights up bluish. Note: The initialization takes about 4 to 5 minutes. After the spectrometer initialization is completed successfully, the spectrometer status indicator turns automatically to blue indicating that the spectrometer is ready to operate. In case the spectrometer status indicator turns to yellow (i.e. warning) or red (i.e. error), first diagnose the cause of the fault and troubleshoot before starting with the measurements. ☞ For information about fault diagnosis and troubleshooting, see chapter 7.
	☞ After having switched on the spectrometer, wait at least 15 minutes before starting the first measurement. This allows for the spectrometer to stabilize. ☞ For high-precision measurements, wait at least two hours to allow the laser to stabilize.	
2		**In case of a PC data station** Switch on the PC and the monitor. After having logged in, the desktop screen appears.
		**In case of the integrated panel PC** The panel PC starts already booting and the touch screen is automatically switched on as soon as the spectrometer is connected to the mains power supply. By default, the OPUS/TOUCH home screen appears.

5.3 Switching off the spectrometer system

1		Switch off the spectrometer using the ON/OFF switch ① at the spectrometer rear side.
2		**In case of a PC data station** Switch off the PC and the monitor.
		**In case of the integrated panel PC** Switch off the integrated panel PC using the ON/OFF switch ① at to top side of the touch screen. Note: To switch on the integrated panel PC, press again the ON/OFF switch ① at to top side of the touch screen. Note: By means of the ON/OFF switch ①, the integrated panel PC can also be set in the standby mode.

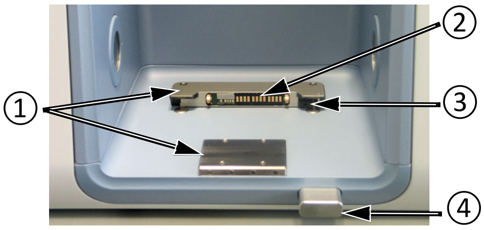
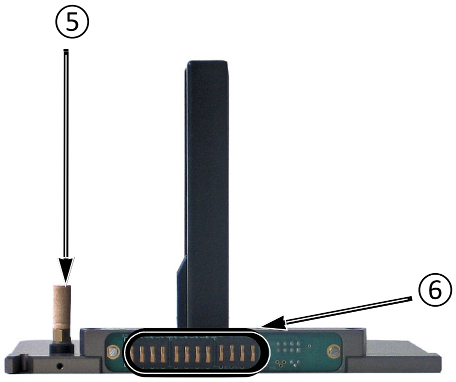
i Switch off the spectrometer only in case of a long time of non-use. We recommend keeping the spectrometer in the on-state overnight and over the weekend. Reason: After being switched on again, the spectrometer is ready for measurement after about 15 minutes. For high-precision measurements, however, a waiting time of about two hours is necessary to allow the thermal spectrometer components to stabilize.

5.4 Placing an accessory in the sample compartment

5.4.1 QuickLock mechanism

Bruker offers a large variety of measurement accessories designed for dedicated applications. For installing these accessories in the spectrometer, the sample compartment is equipped with an accessory locking mechanism called QuickLock. Therefore, only accessories with a QuickLock-baseplate can be used.

The QuickLock locking mechanism allows for a solid lock and a quick and exact positioning of the accessory in the sample compartment. And the available QuickLock-type accessories ensure an exact and reproducible positioning of the sample in the measurement position.

	**Spectrometer sample compartment (inside view)** ① - QuickLock mechanism for locking the accessory ② - Contact strip (electronic connectors for AAR and CAN bus; it is the counterpart to the contact strip at the QuickLock baseplate of the accessory ⑥) ③ - Purge gas inlet (Note: The purge gas inlet provides for purging the sample compartment with dry air or nitrogen gas. With installed accessory, the purge gas enters the sample compartment via the purge gas diffuser ⑤ at the accessory.) ④ - QuickLock button
	**Standard sample holder with QuickLock baseplate** ⑤ - Purge gas diffusor for purging the sample compartment with dry air, if desired ⑥ - Contact strip (electronic connectors for AAR and CAN bus; it is the counterpart to the contact strip at the QuickLock mechanism in the sample compartment ②) Note: This sample holder for transmission measurements is included in the standard delivery scope of the spectrometer.

5.4.2 Putting an accessory in the sample compartment

1		Press the QuickLock button. Put the accessory into the sample compartment with the contact strip of the accessory QuickLock baseplate facing to the contact strip of the QuickLock mechanism in the sample compartment. While inserting the accessory in the QuickLock mechanism, tilt the accessory QuickLock baseplate front edge slightly upwards.
2		Press the QuickLock button for the accessory to lock in place.
3	➢ As soon as the accessory QuickLock baseplate locks in place, the electronic connections for AAR are established. This is indicated by a beep.	

5.4.3 Automatic accessory recognition (AAR)

All QuickLock-type accessories are electronically coded. So, as soon as an accessory locks in place of the spectrometer QuickLock mechanism, it is automatically recognized by the OPUS software program. This software feature is called AAR (Automatic Accessory Recognition). In addition, the OPUS/AAR program performs several predefined OVP tests and loads automatically the corresponding experiment file including the adequate measurement parameter settings and values, provided the user has already defined and stored them for the accessory in question.

Note: When you put a certain accessory in the sample compartment for the very first time, the OPUS/AAR software cannot recognize it because it is not yet registered. In this case, the software prompts you to register the new accessory.

☞ For detailed information about the OPUS software feature AAR, refer to the OPUS Reference Manual. For detailed information about how to define OVP test parameters for certain accessory types, see the Accessory Manager User Manual.

5.4.4 Taking an accessory out of the sample compartment

1		Press the QuickLock button to unlock the accessory.
2		Take the accessory out of the QuickLock mechanism in the sample compartment. Be careful not to damage the contact strips.

5.4.5 Deactivating the automatic shutters

In case the spectrometer is equipped with automatic shutters and the currently installed accessory requires an alignment with the sample compartment being open, you have to deactivate the automatic opening-&-closing-mode of the shutters. Proceed as follows:

1. Start the OPUS program.
2. Select in the OPUS *Measure* menu the *Direct Command Entry* function.
3. *Direct Command Entry* dialog: Enter the direct command *flp=0*. Click on the *Send Command* button.

➢ Thereupon, the shutters move out of the beam path and uncover the sample compartment openings.

4. *Direct Command Entry* dialog: Enter the direct command *fla=0*. Click on the *Send Command* button.

➢ Thereupon, the automatic opening-&-closing-mode of the shutters is deactivated and you can open and close the sample compartment without any shutter movement.

Note: With the direct command *fla=1* you can reactivate the automatic opening-&-closing-mode of the shutters.

☞ For an overview about the direct commands for controlling the shutters, see section 5.8.5.

5.5 Performing a PQ test with OVP

It is highly recommended to validate the spectrometer performance each day before you start your analytical work by performing a PQ test[1] using OVP[2].

Whenever accessories are used, it is essential to check the performance of the spectrometer with installed accessory in addition to the performance of the spectrometer itself. A misaligned accessory, for example, can strongly influence the performance of the analysis system even if the performance of spectrometer itself is OK.

☞ **For detailed information about OVP and how to perform a PQ test refer to the OPUS Reference Manual.**

5.6 General measurement procedure

Generally, a measurement with the spectrometer involves the following basic steps:

	Working step	**Explanations / references**
1	Specify the measurement parameters in OPUS.[1]	☞ The standard parameter settings and values are listed in section C.2. ☞ For detailed information about the measurement parameters, refer to the OPUS Reference manual or OPUS/TOUCH Manual.
2	If you intend to measure the sample using a special accessory, place the accessory (without sample!) in the sample compartment.	☞ For information about how to insert a Quick-Lock-type accessory into the spectrometer sample compartment, see the section 5.4. ℹ Bruker offers a wide range of accessories designed for special analytical applications. For detailed information about how to perform a measurement with a particular accessory, refer to the User Instructions delivered with the accessory in question.
3	Equilibrate purge.	Before starting the background measurement, make sure that the purge has sufficiently removed the water vapor from the IR-beampath. Depending on the geometry and the volume of the accessory optics, the equilibration will take several minutes after an accessory exchange. Note: In case the equilibration of the purge has been insufficient, the sample spectrum will contain water bands. ☞ For information about how to purge, see also section 5.8. ☞ For information about the purge gas requirements and about how to connect the spectrometer to the purge gas supply line, see section 3.7.

---

1. PQ test - Performance Qualification Test
2. OVP - OPUS Validation Program is an integral part of the OPUS software. It is intended for performing spectrometer validation tests like OQ and PQ.

	Working step	Explanations / references
4	In OPUS, start a background measurement (i.e. **without** a sample being in the sample compartment).	ℹ The purpose of the background measurement is to detect the influence of the ambient conditions (level of air humidity, temperature etc.), the auxiliary materials (e.g. solutions), that are required for preparing the sample, and the spectrometer itself on the spectroscopic measurement result. After the subsequent sample measurement, OPUS calculates automatically the result sample spectrum by dividing the sample spectrum (SSC) by the background spectrum (RSC). In doing so, those spectral bands, that result from the ambient conditions, auxiliary materials and/or the spectrometer, are eliminated from the result sample spectrum. ➢ In case you intend to measure the sample with an ATR accessory, perform the background measurement with a sample-free ATR crystal. ➢ Depending on how you intend to prepare your sample (e.g. KBr pellet, Nujol mull or sample solution), it is highly recommended to perform the background measurement with either a pure KBr pellet or the pure nujol or the pure solution placed in the sample position. ☞ For detailed information about sample preparation refer to appendix F.
5	Put the sample in the sample compartment by positioning the sample in the measurement position.	
6	In OPUS, start a sample measurement.	☞ **Important:** Perform both the background measurement and the sample measurement with the same parameter settings in OPUS. Ensure that for both measurements, the ambient conditions (water vapor concentration, temperature etc.) are identical or at least nearly identical. ➢ Afterwards, OPUS calculates automatically the result sample spectrum by dividing the sample spectrum (acquired in step 6) by the background spectrum (acquired in step 4). ☞ For detailed information about the OPUS functions for data acquisition, manipulation and evaluation refer to the OPUS Reference Manual or OPUS/TOUCH Manual.

[1] For performing measurements, the following OPUS software programs are available:

- **OPUS/IR:** This software program is installed on a PC data station (e.g. PC, laptop etc.). For information about OPUS/IR, refer to the OPUS Reference Manual.
- **OPUS/TOUCH:** This software program is installed on the integrated panel PC. For information about OPUS/TOUCH, refer to the OPUS/TOUCH Manual.

5.7 Toggling between the external PC and the integrated panel PC

➢ **Important:** Both the integrated panel PC and the externally connected PC data station must use the same OPUS/IR version to avoid compatibility problems!

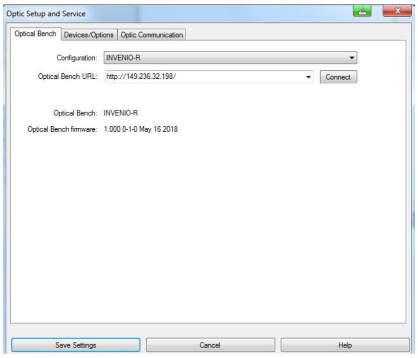
INVENIO with integrated panel PC (optional feature) connected to a PC data station

In this case, the spectrometer can be controlled by both the OPUS/IR software installed on the PC data station and the OPUS/TOUCH software installed on the integrated panel PC.

The spectrometer can be controlled only by one OPUS software program at a time. The user can toggle between them.

Note: To connect the spectrometer with the PC data station, first the user has to disconnect actively the other connection between spectrometer and integrated panel PC or vice versa.

PC data station with OPUS/IR software



Configuration: INVENIO-R
Optical Bench URL: http://149.236.32.198/
Optical Bench: INVENIO-R
Optical Bench firmware: 1.000 0-1-0 May 16 2018

Connecting with the spectrometer

1. PC data station: Start the OPUS/IR software and log into OPUS.
2. Select in the OPUS *Measure* menu the *Optic Setup and Service* function.
3. In the *Configuration* drop-down list, select INVENIO-S.
4. *Optical bench URL*: Enter the IP address of the spectrometer.

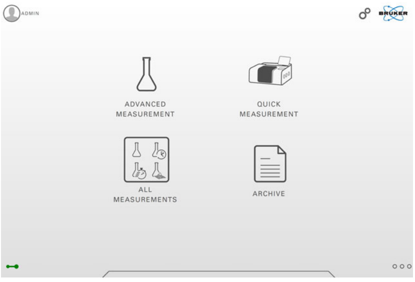
- If the spectrometer is connected directly to an external PC, the standard IP address is 10.10.0.1.
- In case of a DHCP-assigned IP address, you can enter instead of the IP address *invenio-s-SN* with *SN* being the serial number of the spectrometer in question (e.g. *invenio-s-123*). Note: You find the serial number of the spectrometer on the type label at the spectrometer rear side.
- In case the spectrometer is directly connected to a network and a static IP address has been assigned using the FCONF program, you can retrieve the IP address as described in section E.6.

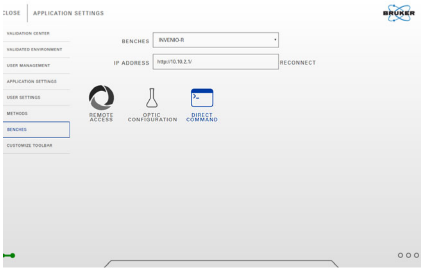
5. Click on the *Connect* button.

Disconnecting

1. Select in the OPUS *Measure* menu the *Optic Setup and Service* function.
2. In the *Configuration* drop-down list, select the option *No optical bench connected*.

Integrated panel PC with OPUS/TOUCH software





BENCHES INVENIO-R

IP ADDRESS http://10.10.2.1/

OPUS/TOUCH provides two variants for connecting with the spectrometer and disconnecting.

1. Conventional variant:

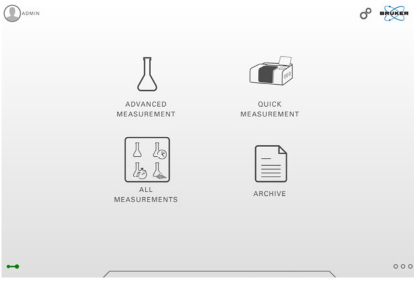
Connecting with the spectrometer

1. OPUS/TOUCH home screen: Tap the ⚙ icon.
2. In the view that opens, tap **BENCHES**.
3. Select the spectrometer and enter the spectrometer IP address.
4. Tap **RECONNECT**.

➢ *If the connection between spectrometer and panel PC has been established, the ●━● icon is shown at the lower left edge of the home screen.*

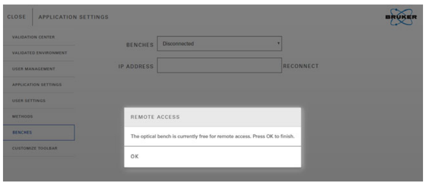
Disconnecting

1. Return to the OPUS/TOUCH home screen.
2. OPUS/TOUCH home screen: Tap the ⚙ icon.
3. In the view that opens, tap **BENCHES**.
4. In the **BENCHES** drop-down list, select **Disconnected**.



BENCHES INVENIO-R

IP ADDRESS http://10.10.2.1/



BENCHES Disconnected

IP ADDRESS

REMOTE ACCESS

The optical bench is currently free for remote access. Press OK to finish.

2. Variant: Disconnecting and reconnecting via Remote Access

Disconnecting

1. OPUS/TOUCH home screen: Tap the ⚙ icon.
2. In the view that opens, tap **BENCHES**.
3. Tap the REMOTE ACCESS icon.

➢ Now the connection between the panel PC and the spectrometer is interrupted and the PC data station can connect with the spectrometer.

Reconnecting

1. As soon as the optical bench is free for access again (i.e. the PC data system has disconnected), you can easily reconnect by tapping OK.

➢ Now the panel PC reconnects with the spectrometer again.

5.8 Purging the spectrometer

5.8.1 General information

The spectrometer provides for purging both the sample compartment and the optical bench (i.e. interferometer and the detector compartment).

Purging the spectrometer with dry air or nitrogen gas reduces the content of unwanted atmospheric interferents like water vapor and carbon dioxide inside the spectrometer significantly. Especially the water vapor in the ambient air absorbs IR radiation. These absorptions are unwanted because they manifest in the spectrum. In the worst case, H_2O bands mask the spectral bands resulting from the sample. Therefore, purging the spectrometer is recommended, especially when you frequently open the sample compartment cover (e.g. due to a sample substitution) and/or if the ambient air has a high water vapor concentration.

When you measure with a purged spectrometer, bear in mind the following: After the measurement, OPUS calculates automatically the result sample spectrum by dividing the measured sample spectrum by the background spectrum (measurement without sample). In doing so, the H_2O and CO_2 bands, that result from the ambient air, are eliminated from the result sample spectrum. Consequently, to get a result sample spectrum that is (almost) free of H_2O and CO_2 bands that result from the air inside the spectrometer, it is not necessary to purge the spectrometer over a long period of time because not the absolute concentration of H_2O and CO_2 inside the spectrometer is important but a constant concentration of these gases during both the background and the sample measurement, i.e. the H_2O and CO_2 concentration inside the spectrometer should be (almost) identical during both measurements.

This can be achieved by proceeding as follows: Before starting the background measurement, simulate a sample exchange (with regard to the duration of the open sample compartment) and a spectrometer purging (with regard to the purge duration before the measurement) as you will do it later for the real sample measurement.

For the above mentioned reason, it is not recommended trying to reduce the H_2O and CO_2 content as far as possible by purging the spectrometer for a long period of time before starting the background measurement because the subsequent sample measurement would require the same long purge period before the sample measurement can be started.

Due to the integrated desiccant cartridges, purging the spectrometer is not necessarily required. However, it is recommended especially when you frequently open the spectrometer compartment. Purging with dry air or nitrogen reduces the water vapor concentration inside the spectrometer within a shorter time than a desiccant cartridge can do. Consequently, purging reduces the waiting time until optimal air conditions inside the spectrometer are reached again.

To maintain the dry air quality in the optical bench (achieved by purging) while the sample compartment is open, the two circular sample compartment openings are closed either by windows or by automatic shutters.

☞ For information about how the automatic shutters work, see section 5.8.4.

☞ For information about how to control the shutters, see section 5.8.5.

5.8.2 Purge gas supply requirements

Purge the spectrometer, for example, with dry air or low pressure nitrogen gas. The purge gas supply has to meet the following requirements:

- dry air or nitrogen gas (dew point < -40°C corresponds to a degree of dryness of 128ppm humidity)
- oil-free and dust-free
- max. pressure: 0,5 bar (7.25 psi)

5.8.3 Controlling the purge gas flow rate

When the spectrometer is purged continuously the recommended flow rate is 200 liters/hour. Make sure that the flow rate does not exceed 500 liters/hour.

Adjust the purge gas flow rate using an air flow regulator.

i Bruker offers an air flow regulator (option S316/7).

5.8.4 Shutters - Automatic mode of operation

The automatic shutters isolate the sample compartment from the rest of the spectrometer (optical bench). The purpose of the shutters is to maintain the dry air quality in the optical bench (achieved by purging) while the sample compartment is open (e.g. for exchanging the sample).

As soon as you lift the sample compartment cover, the shutters close automatically. When you close the sample compartment, the shutters open again with a time delay of about 5 seconds.

5.8.5 Controlling the shutters

You can control the shutters as follows:

1. Start the OPUS software.
2. Select in the *Measure* menu the *Direct Command Entry* function.
3. In the *Direct Command Entry* dialog, enter the corresponding direct command. See the following table.

Direct command	Executed command
flp=0	The shutters move out of the beampath and uncover the sample compartment openings.
flp=1	The shutters move in the beampath and close the sample compartment openings.
fla=0	This command deactivates the automatic opening-&-closing-mode.
fla=1	This command activates the automatic opening-&-closing-mode.

4. Click on the *Send Command* button.

5.9 Exchanging a DigiTect-type detector

5.9.1 General information

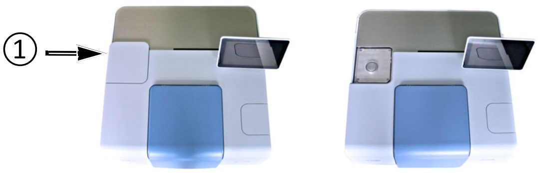
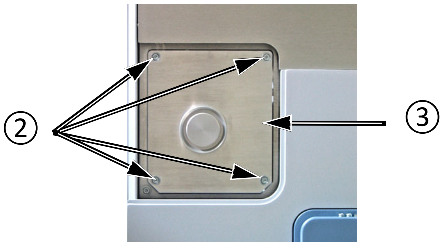
For installing a DigiTect-type detector, there is an additional detector position (B in fig. 4.6) which is an optional feature. In case your measurement requires a different spectral range and/or another detection sensitivity than the standard detector[1] allows, you can install a DigiTect-type detector, such as a MCT detector with a higher sensitivity, for example.

☞ In section 4.5.3, all available optional detectors are listed including their detection sensitivity and the spectral range they cover.

5.9.2 Procedure

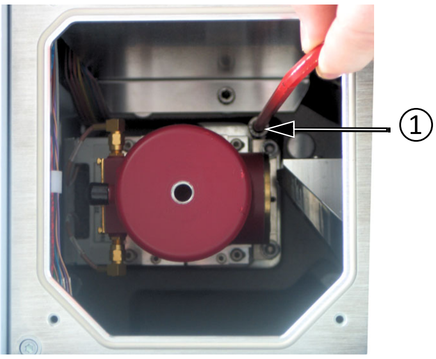
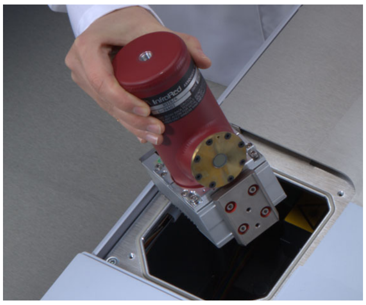
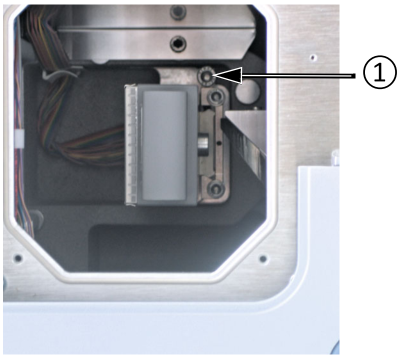
	**Required tools** • TORX screw driver Note: This tool is included in the delivery scope of the spectrometer. • Hex key (size: 6 mm) Note: These tools are included in the delivery scope of the DigiTect-type detector.

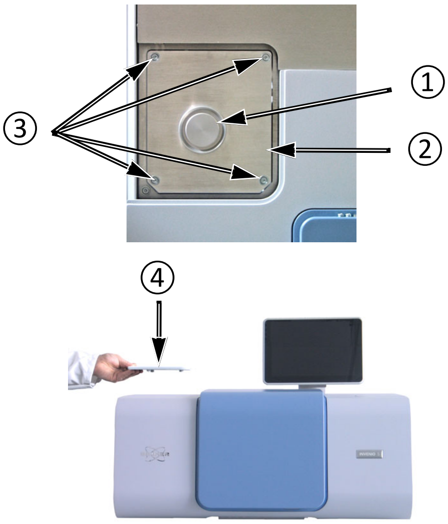
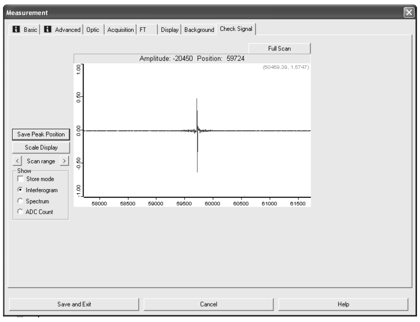
The optionally available detectors are mounted on a dovetail slide which allows an easy exchange. A re-alignment is not necessary.

1		**To gain access to the detector:** 1. Remove the plastic cover ①. Note: This cover is held in place magnetically.
		2. Loosen the four TORX screws ② and remove the metallic cover ③.

---

[1] The standard detector is a DLaTGS detector with KBr window for measurements in the mid-infrared region.

2	 	**To remove the detector:** 1. Loosen the locking screw ① (Allen screw). Use the supplied hex key (size 6 mm). 2. Take the detector straight upwards out of the dovetail guide. **Caution:** Remove the detector carefully in order not to damage the detector and/or the mirrors which are installed in the detector compartment.
3		**To install the exchange detector:** 1. Insert the exchange detector precisely into the dovetail guide and push the detector downwards until you feel a resistance. **Caution:** Insert the detector carefully in order not to damage the detector and/or the mirrors which are installed in the detector compartment. 2. Fasten the Allen screw ① using the supplied hex key (size 6mm). ➢ A beep indicates that the detector has been recognized by the electronics. The electrical connections are established automatically.

4		**To close the spectrometer:** Note: In case an MCT detector is installed, the blind cap ① needs to be removed first. 1. Put the metallic cover ② in place and fasten the four screws ③. 2. Put the plastic cover ④ in place. Note: This cover is held in place magnetically. Ensure that it is positioned correctly.
5	 Amplitude: -20450 Position: 59724 ☐ Store mode ● Interferogram ○ Spectrum ○ ADC Count	**To check the signal:** Open the OPUS software program and check whether a signal is detected and whether the signal intensity is OK. ☞ For information about how to check the signal, see section 5.10.

5.10 Checking the signal

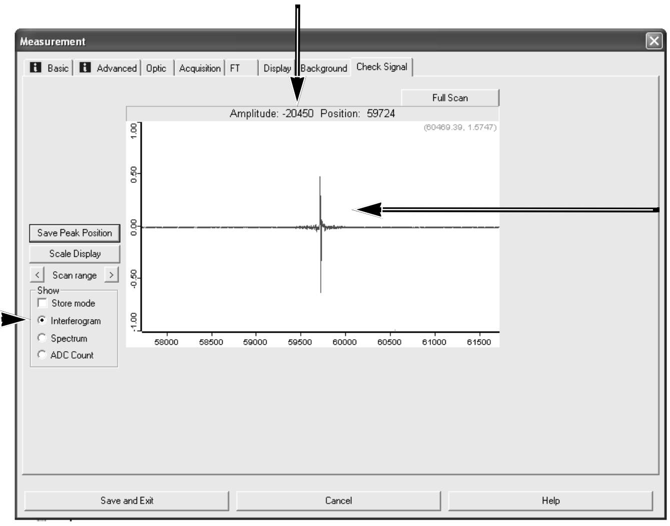
5.10.1 General information

Especially after you have replaced a spectrometer component (e.g. source, detector), it is advisable to check whether a signal is detected and to check whether the signal intensity (signal amplitude) is sufficient.

5.10.2 Procedure

1. Make sure that there is not any accessory and/or sample in the spectrometer sample compartment.
2. Open the software program OPUS.
3. Select in the *Measure* menu the *Advance Measurement* function.
4. Click in the *Measurement* dialog window on the *Check Signal* tab.
5. Make sure that the *Interferogram* option button is activated. (See fig. 5.1.)

The amplitude value indicates the signal intensity that is currently detected.



Amplitude: -20450 Position: 59724

☐ Store mode
● Interferogram
○ Spectrum
○ ADC Count

The interferogram indicates that a signal is detected.

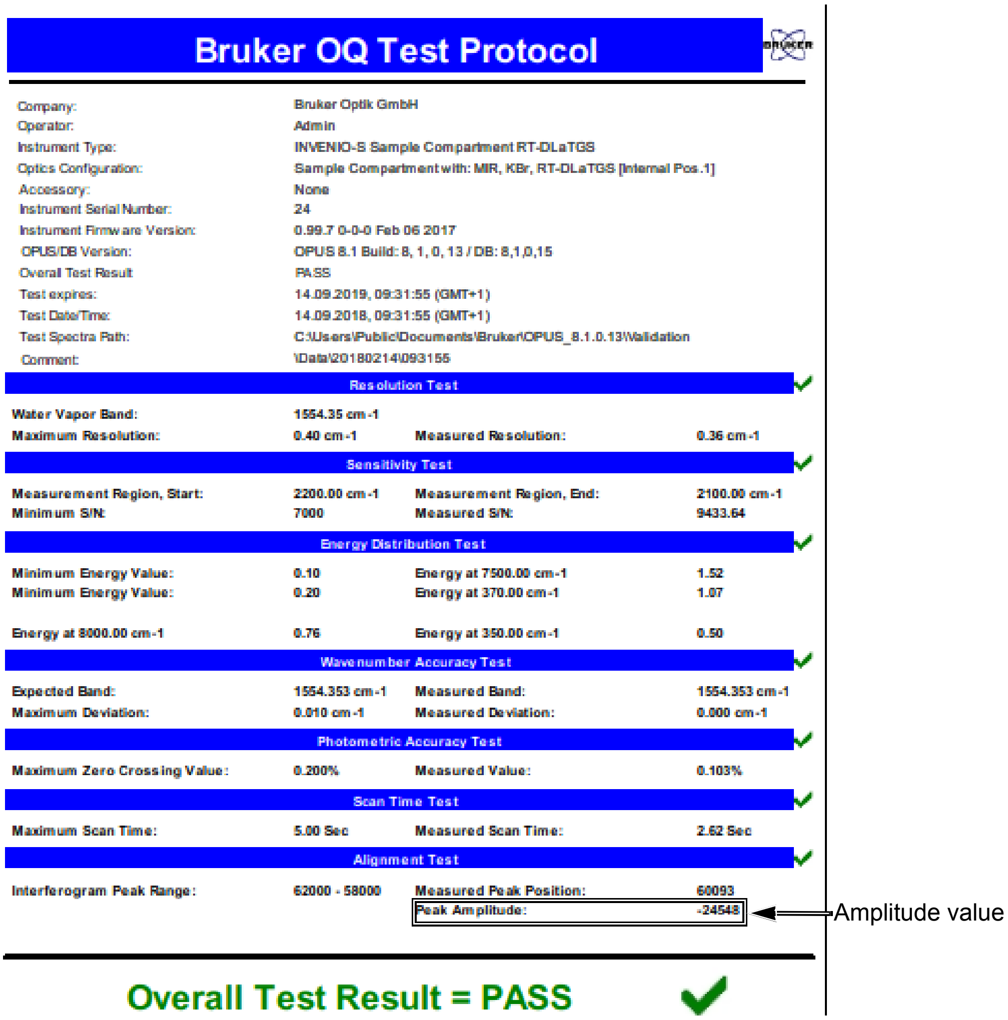
Interferogram option button (activated)

Figure 5.1: OPUS Dialog Window - *Measurement*

For verifying the currently detected signal intensity, compare the amplitude value displayed in OPUS (fig. 5.1) with the amplitude value stated in the supplied OQ test protocol[1]. (See fig. 5.2.)

---

[1] The supplied OQ test protocol documents the result of a factory-performed OQ test. The test has been performed with the spectrometer components being optimally adjusted. You will find the OQ test protocol in the folder supplied with the spectrometer.



Bruker OQ Test Protocol

Company:	Bruker Optik GmbH
Operator:	Admin
Instrument Type:	INVENIO-S Sample Compartment RT-DLaTGS
Optics Configuration:	Sample Compartment with: MIR, KBr, RT-DLaTGS [Internal Pos.1]
Accessory:	None
Instrument Serial Number:	24
Instrument Firmware Version:	0.99.7 0-0-0 Feb 06 2017
OPUS/DB Version:	OPUS 8.1 Build: 8, 1, 0, 13 / DB: 8,1,0,15
Overall Test Result	PASS
Test expires:	14.09.2019, 09:31:55 (GMT+1)
Test Date/Time:	14.09.2018, 09:31:55 (GMT+1)
Test Spectra Path:	C:\Users\Public\Documents\Bruker\OPUS_8.1.0.13\Validation
Comment:	\Data\20180214\093155

Resolution Test ✓

Water Vapor Band:	**1554.35 cm-1**		
Maximum Resolution:	**0.40 cm-1**	**Measured Resolution:**	**0.36 cm-1**

Sensitivity Test ✓

Measurement Region, Start:	**2200.00 cm-1**	**Measurement Region, End:**	**2100.00 cm-1**
Minimum S/N:	**7000**	**Measured S/N:**	**9433.64**

Energy Distribution Test ✓

Minimum Energy Value:	**0.10**	**Energy at 7500.00 cm-1**	**1.52**
Minimum Energy Value:	**0.20**	**Energy at 370.00 cm-1**	**1.07**
Energy at 8000.00 cm-1	**0.76**	**Energy at 350.00 cm-1**	**0.50**

Wavenumber Accuracy Test ✓

Expected Band:	**1554.353 cm-1**	**Measured Band:**	**1554.353 cm-1**
Maximum Deviation:	**0.010 cm-1**	**Measured Deviation:**	**0.000 cm-1**

Photometric Accuracy Test ✓

Maximum Zero Crossing Value:	**0.200%**	**Measured Value:**	**0.103%**

Scan Time Test ✓

Maximum Scan Time:	**5.00 Sec**	**Measured Scan Time:**	**2.62 Sec**

Alignment Test ✓

Interferogram Peak Range:	**62000 - 58000**	**Measured Peak Position:**	**60093**
		Peak Amplitude:	**-24548**

Amplitude value

Overall Test Result = PASS ✓

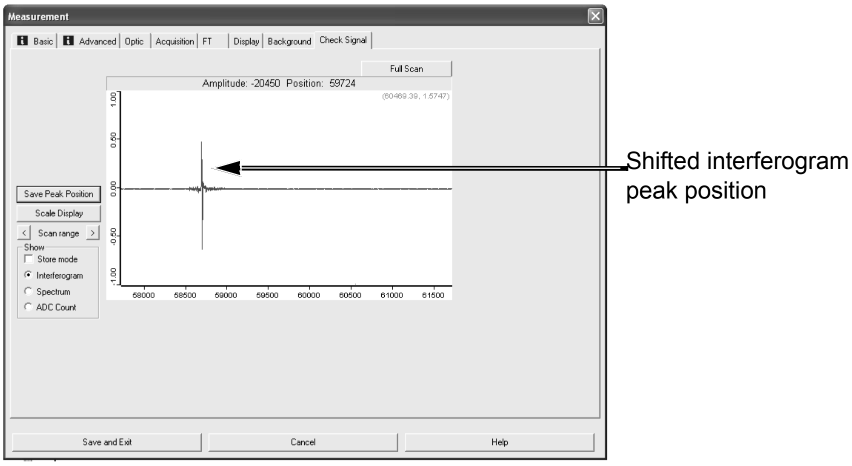
Figure 5.2: OQ- Test Protocol

If there is not any signal detected or if the amplitude value displayed in OPUS (fig. 5.1) deviates significantly from amplitude value of the supplied OQ test protocol (fig. 5.2) check the installation of the spectrometer component(s) you have replaced before. For troubleshooting, see also section .7.5.4

5.10.3 Saving the interferogram peak position

General information

If the interferogram peak position has shifted in the course of time (i.e. it is no longer in the center of the display as shown in fig. 5.3), you have to save the new peak position.



Amplitude: -20450 Position: 59724

☐ Store mode
● Interferogram
○ Spectrum
○ ADC Count

Shifted interferogram peak position

Figure 5.3: OPUS Measurement dialog - Check Signal dialog page

➢ Note: A shifted interferogram peak position is also indicated by the message *Peak Position out of range* in OPUS. This information message appears when you start a measurement with the interferogram peak position being shifted.

Procedure

1. Open the software program OPUS.
2. Select in the *Measure* menu the *Advance Measurement* function.
3. Click in the *Measurement* dialog window on the *Check Signal* tab.
4. Activate the *Interferogram* option button if it is not already activated.
5. Press the *Save Peak Position* button.
6. Exit the dialog.

➢ Note: When you reopen the *Check Signal* dialog page, the interferometer peak position is now in the center of the display.

5.11 Cooling a detector with liquid nitrogen

5.11.1 General information

Optionally, several detectors are available which require cooling (e.g. MCT detectors). See section 4.5.3.

The operating temperature of these detectors is significantly below room temperature. To achieve the required operating temperature, the detector needs to be cooled with liquid nitrogen, i.e. liquid nitrogen is filled in the detector.

The hold time indicates how long the cooling effect of the liquid nitrogen lasts. To ensure an optimum signal detection, the detector needs to be filled with liquid nitrogen in regular intervals. The available liquid nitrogen-cooled detectors have different nominal hold times: 8, 12, or 24 hours.

Indications of a weakened or disappeared cooling effect are a low signal intensity or no signal detection.

☞ For information about how to check the signal, see section 5.10.

In case no signal is detected, the OPUS status lamp turns to red. This problem is also indicated by the following instrument status message in OPUS: *Detector not ready.*

☞ See also section 7.2.3.

If the actual hold time of a liquid nitrogen-cooled detector is considerably shorter than the nominal hold time, the detector dewar needs to be evacuated.

☞ For information about how to evacuate the detector dewar, see section 6.3.

5.11.2 Safety notes

The temperature of liquid nitrogen is minus 196°C.

⚠ CAUTION

Risk of frostbites due to improper handling of liquid nitrogen

Non-observance of the following safety instructions may result in an injury.

➢ **Avoid skin contact.** Handle liquid nitrogen always with care.

➢ **Protect your eyes by wearing a face shield or safety goggles!** Also the gases escaping from the liquid nitrogen are extremely cold and can cause frostbite. The delicate eye tissue can be damaged if exposed to this cold gas even for a short time. Note that goggles without side shields do not provide adequate protection!

⚠ CAUTION

Risk of asphyxiation due to lack of oxygen

Non-observance of the following safety instructions may cause health problems.

➢ **Use liquid nitrogen only in well-ventilated areas!** High nitrogen gas concentrations in an enclosed area can cause asphyxiation! Note: Nitrogen gas is colorless, odorless and tasteless. Therefore, it can not be detected by human senses and will be inhaled as if it were normal air.

5.11.3 Preparing the detector compartment cover for funnel insertion

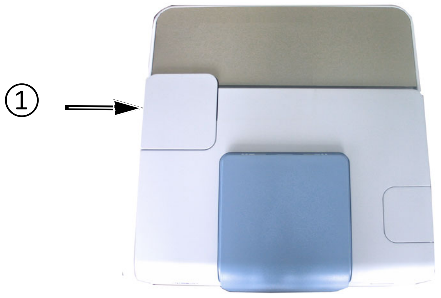
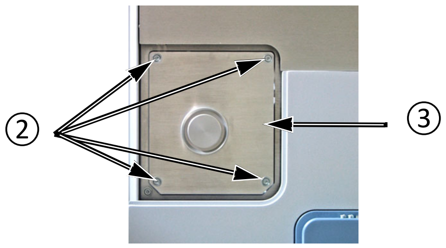
General information

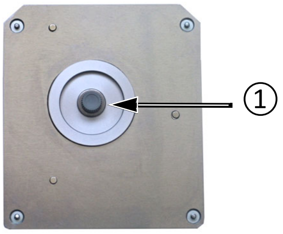
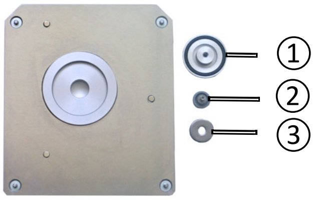
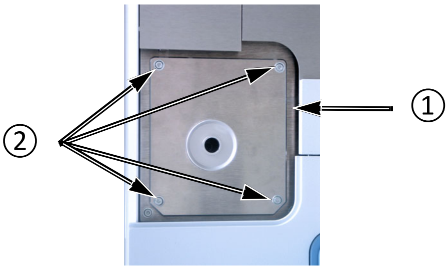
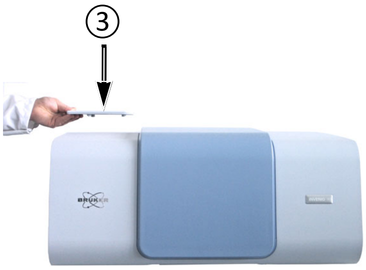
In case the liquid nitrogen-cooled detector has been delivered together with the spectrometer, the detector compartment cover is already prepared for the funnel insertion. If the detector has been ordered at a later date you need to prepare the detector compartment cover as described below.

Required tool

	**Required tool** - TORX screw driver Note: This tool is included in the delivery scope of the spectrometer.

Procedure

1	  	**To gain access to the detector:** 1. Remove the plastic cover ①. Note: This cover is held in place magnetically. 2. Loosen the four TORX screws ② and remove the metallic cover ③.

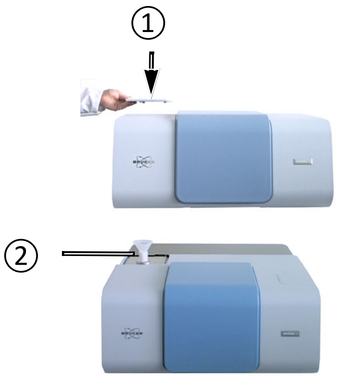
2		Turn the detector compartment cover upside down and remove the cap from the filling hole. To do this, screw off the knurled screw ①and remove the complete closure assembly.
		The closure assembly consists of the following items: ① - cap ② - knurled screw ③ - washer
3		**Attention:** Before closing the detector compartment, make sure that the bellows-type sealing adapter ① is screwed on the MCT detector. Otherwise, when you fill liquid nitrogen in the detector dewar using the funnel, it will flow into the detector compartment and cause serious damage! **Note:** The MCT detector is delivered with a bellows-type sealing adapter. By default, the sealing adapter is factory-mounted. If not, screw the sealing bellows on the filling piece of the MCT detector.
4	 	1. Put the metallic cover ① in place and fasten the four TORX screws ②. 2. Put the plastic cover ③ in place. Note: This cover is held in place magnetically. Ensure that it is positioned correctly.

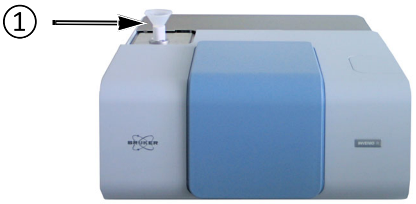
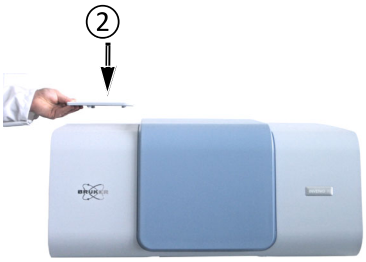
5.11.4 Filling liquid nitrogen into the detector

Required equipment and consumables

- Funnel (It is included in the delivery scope of the liquid nitrogen-cooled detector.)
- Liquid nitrogen
- Safety goggles with side shields (recommended safety equipment)

Procedure

1		1. Remove the plastic cover ①. Note: This cover is held in place magnetically. 2. Insert the funnel ②.
2		Pour slowly liquid nitrogen in the funnel. Avoid spilling the liquid on the spectrometer housing. At first the liquid nitrogen evaporates and streams out again. Wait until the funnel is empty before refilling. When the liquid nitrogen stops streaming out, the detector dewar has reached the liquid nitrogen temperature. Then, pour again liquid nitrogen in the funnel. Repeat this procedure until the detector has been filled to maximum. (As a rough rule of thumb for the standard MCT detector: the maximum capacity is about the quantity of two to three funnel fillings. Note that the first two funnel fillings will evaporate almost completely.) **Avoid overfilling!** In this case the liquid flows out of the filling port.
	Caution: Liquid nitrogen boils and splashes when it is filled in a warm container. Especially at the beginning, when the temperature difference between the detector dewar and the liquid nitrogen is still very large, the liquid nitrogen may squirt out forcefully due to the boiling delay. Therefore, observe the following safety instructions: ➢ Fill in the liquid nitrogen slowly to minimize boiling and splashing. ➢ **Stand clear of boiling and splashing liquid nitrogen and its issuing gas! Wear safety goggles or a face shield.** ➢ Be aware that during the entire filling process, liquid nitrogen can squirt out of the detector dewar from time to time.	

3	 	After having filled in sufficient liquid nitrogen, take the funnel ① out of the filling hole and ... . put the plastic cover ② in place. Note: This cover is held in place magnetically. Ensure that it is positioned correctly.
4	➢ Wait about 20 minutes before starting a measurement to allow the detector to stabilize thermally.	

5.12 Measurements with the integrated ATR unit

5.12.1 Handling instructions

- **IMPORTANT: Read carefully the following notes on how to avoid ATR crystal damages before using the ATR unit for the first time. Note that Bruker Optik GmbH does not provide warranty for use-related crystal damages caused by improper handling! Moreover, spectroscopic measurements performed with a damaged ATR crystal do NOT yield reliable results!**

To avoid damages, observe the following notes:

NOTE

- For applying pressure on solid samples use only the pressure application device and the anvil of the ATR unit. Do not use any modified or custom-made pressure application devices.
- When pressing the sample against the ATR crystal surface, do not exceed the factory-set contact pressure limit value, for example with additional manual force.
- When measuring corrosive chemicals (e.g. strong acids, strong leaches or organic solvents) apply only the minimal required sample amount on the crystal plate and limit the time of exposure to a minimum, i.e. apply the substance on the crystal plate only shortly before you start the measurement and remove it immediately after the measurement. Clean the ATR unit immediately afterwards.

☞ For information about how to clean the ATR crystal plate, see section 5.12.7.

5.12.2 Potential risks and hazards in case of the heatable variant only

During operation, the crystal plate including the ATR crystal of the heatable ATR unit can become hot, max. 80°C. Due to this, there are the following potential risks and hazards:

Risk of burns

⚠ CAUTION

Risk of burns due to hot surfaces

Non-observance of the following safety notes may result in minor or moderate (reversible) injury.

- Do not touch the ATR crystal plate if it is hot. Risk of minor skin burns.
- Before removing a sample from the crystal plate or placing a sample on the crystal plate, wait until the crystal plate has cooled down sufficiently.
- Do not clean the ATR crystal plate until the crystal plate has cooled down sufficiently.

Health hazard due to harmful gases and vapors

⚠ WARNING

Health hazard due to heating up a corrosive or harmful sample

Non-observance of the following safety notes could result in death or serious (possibly irreversible) injury.

➢ Heating up corrosive substances or substances which are hazardous to health can produce toxic or corrosive gases or vapors. Avoid inhaling them. Extract these gases and vapors!

Risk of fire

⚠ WARNING

Risk of fire

Non-observance of the following safety notes could result in death or serious (possibly irreversible) injury and major property damage.

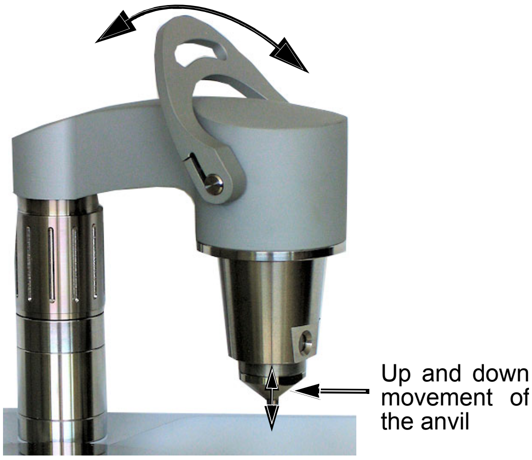
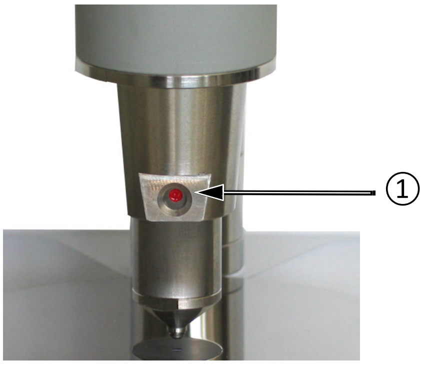
➢ Heating up highly flammable samples involves the risk of fire. Do not heat up those samples above their burning point.

5.12.3 Operating the ATR unit

☞ For information about the operating elements of the pressure application device, see section 4.7.1.

5.12.3.1 Operating the anvil

To achieve the required intimate contact between the sample and the ATR crystal, solid samples[1] need to be pressed against the ATR crystal by means the anvil. The anvil is lifted or lowered by means of the lever.

Directions of lever movement for operating the anvil  	• The operator has put the lever in the back position. → Anvil is the upper position. → No contact pressure is applied on the sample. • The operator has put the lever in the front position → Anvil is in the lower position. → The anvil presses the sample against the ATR crystal.
 	➢ Note: The applied contact pressure is optimal when the red spot is in the center of hole ①.

NOTE

➢ Do NOT try increase the contact pressure any further by additionally exerting force! Otherwise the ATR crystal might be damaged irreversibly! The factory setting is sufficient.

---

[1] Note: Liquids, pastes and gels do not need to be pressed against the ATR crystal.

5.12.3.2 Adjusting the height of the complete pressure application device

① - Pressure application device

② - Rotary knob for adjusting the height of the pressure application device

Rotating the knob ② clockwise moves the pressure application device ① upwards, i.e. the distance between anvil and ATR crystal increases.

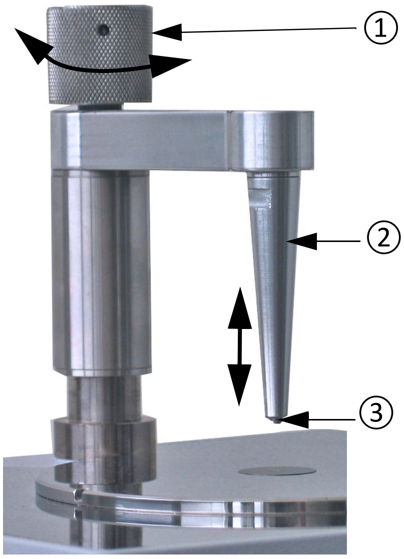
Rotating the knob ② counterclockwise moves the pressure application device ① downwards, i.e. the distance between anvil and ATR crystal decreases.

A height adjustment of the pressure application device is required in the following situations:

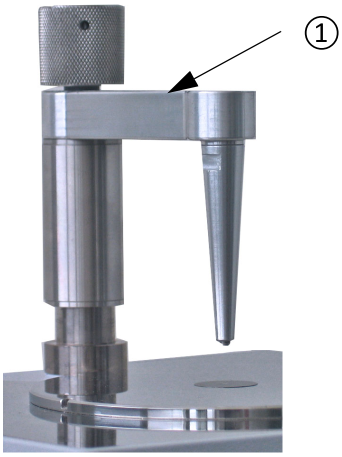
- You have lowered the anvil completely by putting the lever in the front position, but the anvil does yet not contact the sample. In this case you have to lower the complete pressure application device. To do this, turn the height adjustment knob counterclockwise.
- You do not succeed in putting the lever in the front position because the sample is too thick with regard to the currently set height of the pressure application device. (Note: For measurements with the ATR unit, the sample thickness should not exceed 20 mm.) In this case, you have to increase the height of the complete pressure application device. To do this, turn the height adjustment knob clockwise until you succeed in putting the lever in the front position and the red spot is in the center of the hole.

5.12.4 Operating the ATR unit (high-pressure variant)

☞ For information about the operating elements of the pressure application device, see section 4.7.2.

<table>
<tr>
<td>
</td>
<td>

- Rotating the knob ① clockwise ──► The pressure arm ② moves downwards. ──► The anvil ③ presses the sample against the ATR crystal.
- Rotating the knob ① counter-clockwise ──► The pressure arm ② moves upwards. ──► The contact pressure is released.

i The pressure application device is equipped with a slip-clutch mechanism which is activated as soon as the optimal contact pressure is achieved. Further rotating the knob, which is then only possible by a substantial exertion of force, does not further increase the contact pressure.
</td>
</tr>
<tr>
<td>
</td>
<td>
The pressure arm ① is rotatable by 360°. For sample exchange or cleaning purposes, it can be swiveled out of the measurement position.

i When you swivel the pressure arm back into the measurement position, the pressure arm snaps into place exactly above the ATR crystal.
</td>
</tr>
</table>

5.12.5 Defining the measurement parameters in OPUS

5.12.5.1 General information

Before starting a measurement, you have to define the measurement parameters including the desired sample temperature using the OPUS software. To do this, proceed as follows:

1. Open the OPUS software program.
2. Select in the OPUS *Measure* menu the *Setup Measurement Parameters* function.
3. Load an adequate XPM-file.
   (Note: For a measurement with the ATR unit, you can use the delivered file *MIR_ATR.XPM*. The default path for this type of files is *C:\Users\Public\Public Documents\Bruker\[OPUS_version]\XPM*.)
4. In the *Setup Measurement Parameters* dialog, define the measurement parameters and the desired sample temperature.

☞ For detailed information about the measurement parameters, refer to the OPUS Reference Manual. For information about how to set the desired sample temperature, see the following section 5.12.5.2.

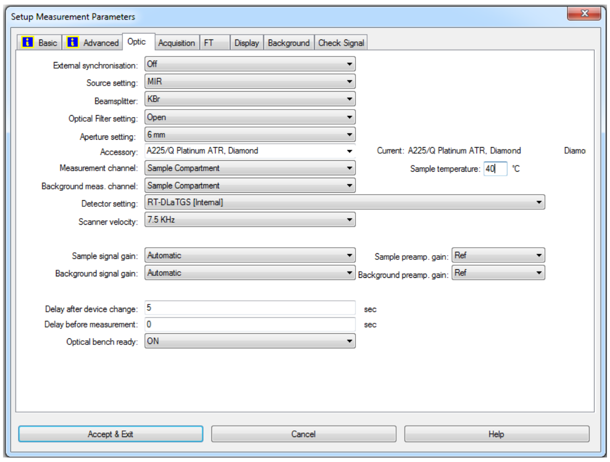
5. After having setup all parameters, click on the *Accept & Exit* button.

➣ The selected parameter settings and values are stored in the XPM-file.

5.12.5.2 Setting the desired sample temperature (in case of the heatable variant only)

The heatable ATR unit allows for heating up the sample at a certain temperature. The sample can be heated up to max. 80°C. To set the desired sample temperature, proceed as follows:

1. In the *Setup Measurement Parameters* dialog, click on the *Optics* tab.
2. Enter the desired sample temperature. (Note: Enter a value which is at least 5° higher than room temperature to ensure that the unit starts to heat. The max. possible temperature is 80°C.)
3. Select in the *Optical bench ready* drop-down list the option *ON,* to ensure that the measurement does not start before the set temperature is reached.



External synchronisation: Off
Source setting: MIR
Beamsplitter: KBr
Optical Filter setting: Open
Aperture setting: 6 mm
Accessory: A225/Q Platinum ATR, Diamond
Current: A225/Q Platinum ATR, Diamond
Diamo
Measurement channel: Sample Compartment
Sample temperature: 40 °C
Background meas. channel: Sample Compartment
Detector setting: RT-DLaTGS [Internal]
Scanner velocity: 7.5 KHz
Sample signal gain: Automatic
Sample preamp. gain: Ref
Background signal gain: Automatic
Background preamp. gain: Ref
Delay after device change: 5 sec
Delay before measurement: 0 sec
Optical bench ready: ON

Figure 5.4: Setting the sample temperature in OPUS

Starting the heating (in case of the heatable variant only)

To start the heating of the ATR unit, proceed as follows:

1. Select in the OPUS *Measure* menu a measurement function (e.g. the *Advanced Measurement* function).
2. Load the XPM file which contains the parameter settings - including the desired sample temperature setting - you have defined for this measurement.
3. The ATR unit starts to heat when you click in the *Measurement* dialog on either:
   - the *Background Single Channel* button or
   - the *Sample Single Channel* button or
   - the *Check Signal* tab

➢ Afterwards, the ATR unit starts to heat until the defined sample temperature is reached. Then, this temperature is maintained.

Note: The background measurement or sample measurement does not start until the defined sample temperature is reached, provided that you have activated the parameter *Optical bench ready.*

Deactivating the heating (in case of the heatable variant only)

To deactivate the heating of the ATR unit, proceed as follows:

1. Select in the OPUS *Measure* menu a measurement function (e.g. the *Advanced Measurement* function).
2. In the *Measurement* dialog, click on the *Optics* tab.
3. For the *Sample Temperature* parameter, enter the value -300.
4. The heating is deactivated when you click in the *Measurement* dialog on either:
   - the *Background Single Channel* button or
   - the *Sample Single Channel* button or
   - the *Check Signal* tab.

5.12.6 Performing a measurement - General procedure

➢ **Note:** To check whether the spectrometer really achieves the specified performance values, it is highly recommended to perform an PQ test[1] each day before you start your analytical work. The PQ test is performed with OVP[2]. For detailed information about how to perform a PQ test, refer to the OPUS Reference Manual.

A measurement with the ATR unit involves the following basic steps:

	Working step	**Explanations / references**
1	Define the measurement parameters. In case of the heatable variant, define also the desired sample temperature in OPUS.	☞ For detailed information about the measurement parameters, refer to the OPUS Reference Manual. ☞ For information about how to set the desired sample temperature, see section 5.12.5
2	Clean the ATR unit.	☞ For information about how to clean the crystal plate, see section 5.12.7.
3	Perform a background measurement using OPUS.	Before starting the background measurement, make sure that: [1] no sample is on the ATR crystal and [2] the anvil is not pressed on the ATR crystal but in the upper position. To start the background measurement, click in the OPUS *Measurement* dialog on the *Background Single Channel* button.
4	Wipe the ATR crystal once again using a paper towel. Afterwards, check the ATR crystal for cleanliness using the OPUS software.	☞ For information about how to check the ATR crystal for cleanliness, see section 5.12.8.
5	Place the sample on the ATR crystal.	Position the sample in the center of the crystal plate. Make sure that the ATR crystal is covered completely with sample material. Due to the small crystal surface, only a small amount of sample material is required. ➢ Note: If you do not succeed in putting the sample on the ATR crystal because there is not sufficient space between the ATR crystal and the anvil you have to increase the height of the complete pressure application device first. For information about how to do this, see section 5.12.3.2.

---

[1] PQ test - Performance Qualification Test

[2] OVP (OPUS Validation Program) is integral part of the OPUS software. It is designed for performing spectrometer qualification tests, namely PQ tests and OQ (Operational Qualification) tests.

	Working step	**Explanations / references**
6	Press the sample against the ATR crystal. Note: Only solid samples (e.g. powder, polymers etc.) need to be pressed against the ATR crystal, liquids and pastes do not!	Press the solid sample against the ATR crystal by putting the lever in the front position. Note: The contact pressure is optimal when the red spot is in the center of the hole as shown in the lower image of fig. 4.9. ☞ For information about how to press the sample against the ATR crystal, see section 5.12.3.1. In case of the high-pressure variant, see section 5.12.4. Note: If the sample is not pressed against the ATR crystal although you have put the lever in the front position, you first have to lower the complete pressure application device sufficiently. ☞ For information about how to lower the complete pressure application device, see section 5.12.3.2.
7	Check the sample signal intensity.	Before you start the sample measurement, it is advisable to check in the live preview whether the sample signal intensity is OK. (Note: For the display of the live preview, the *Display single scans before measurement* check box on the *Display* dialog page needs to be activated. This is the default setting.) On the *Basic* dialog page, click on the *Sample Single Channel* button. Thereupon, the live preview spectrum is displayed. Hint: If the signal intensity is too weak (e.g. in case of a coarse-grained powder), release the contact pressure by putting the lever of the pressure application device in the back position and rearrange the powder on the ATR-crystal. Then press the powder again against the ATR crystal.
8	Start the sample measurement.	To start the sample measurement, click on the *Start Measurement* button below the live preview. Note: After you have started the sample measurement, OPUS waits until the set sample temperature is achieved before it starts the measurement, provided that you have activated the parameter *Optical bench ready.*

	Working step	Explanations / references
		⚠ **WARNING** Non-observance of the following safety notes could result in serious (possibly irreversible) injury. ➢ When measuring highly flammable and/or explosive substances, wear eye-protective glasses! Do not heat up a highly flammable sample above its flash point. ➢ In case of volatile substances, do NOT inhale the vapor! We recommend to use the optional cover for volatile liquids. (See section 5.12.10.1.) ➢ Observe the safety instructions relevant to the hazardous substance in question.
		➢ **Important:** Perform both the background measurement and the sample measurement with the same parameter settings in OPUS. Ensure that for both measurements, the ambient conditions are identical or at least nearly identical. ➢ Afterwards, OPUS calculates automatically the result sample spectrum by dividing the sample spectrum (acquired in step 8) by the background spectrum (acquired in step 3). The result sample spectrum is displayed automatically in OPUS.
9	Remove the sample from the ATR crystal.	In case of a solid sample, first release the sample by lifting the anvil. ➢ **Attention:** After the measurement, remove the sample immediately from the ATR crystal. Keep in mind that certain samples may impair the ATR crystal and / or discolor the crystal plate when they remain on the ATR unit over a longer period of time.
10	Clean the ATR crystal, the sampling surface and the anvil thoroughly.	☞ For information about cleaning the ATR unit, see section 5.12.7.

5.12.7 Cleaning the ATR crystal plate

General information

After **EACH** sample measurement, clean the ATR crystal, the complete sampling surface and the anvil **thoroughly**. Otherwise, sample residues may falsify the result of the following measurement(s).

Clean the ATR unit immediately after the sample measurement to prevent possible sample residues from sticking on the ATR crystal. Dried-up sample residues are more difficult to remove.

Cleaning agents

For cleaning the ATR unit, you can use the following cleaning agents and solvents:

- Ethanol
- Isopropanol
- Water

Use an adequate cleaning agent. The adequacy of a cleaning agent depends mainly on the sample that has been analyzed with the ATR unit.

NOTE

➢ Do **NOT** use caustic or abrasive substances or strong acids! These substances may damage the ATR crystal plate. **Bruker does not provide warranty for use-related crystal damages cause by improper handling!**

i For cleaning the ATR crystal plate, we recommend using a soft cleaning tissue which can be ordered by Bruker. For the order number, see section B.3

Procedure

	1. Pivot the pressure application device out of the measurement position. ➢ Note: The pressure application device is pivotable by 360°. When you pivot the pressure application device in the measurement position, it snaps into place exactly above the ATR crystal.

2. Apply the cleaning agent on all sample contact surface (ATR crystal, crystal plate and anvil) using a soft wipe or a cotton swab.
3. Rub the contaminated surfaces carefully using a lint-free wipe or a non-abrasive paper towel until all residues of the previous sample and contamination are removed.

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i For a gentle and effective cleaning of the ATR crystal surface, we recommend using the special ATR cleaning wipes offered by Bruker. (Order number: 1008033)

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4. Wipe off all cleaning agent residues from the ATR crystal surface, the sample contact surface and the anvil using a dry and non-abrasive paper towel or a soft wipe.

5.12.8 Checking the ATR crystal for cleanliness

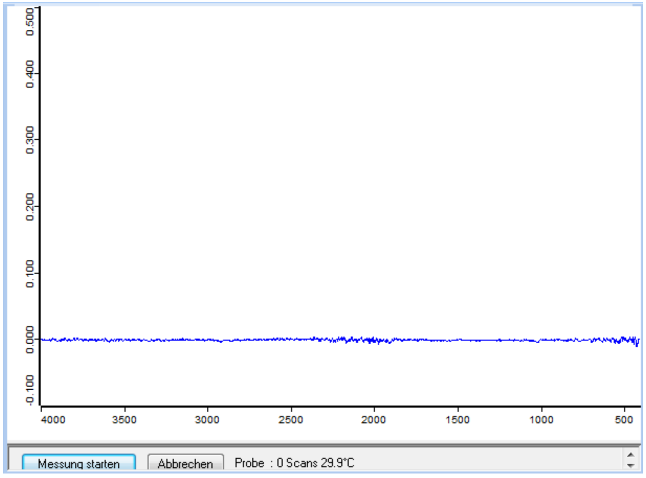
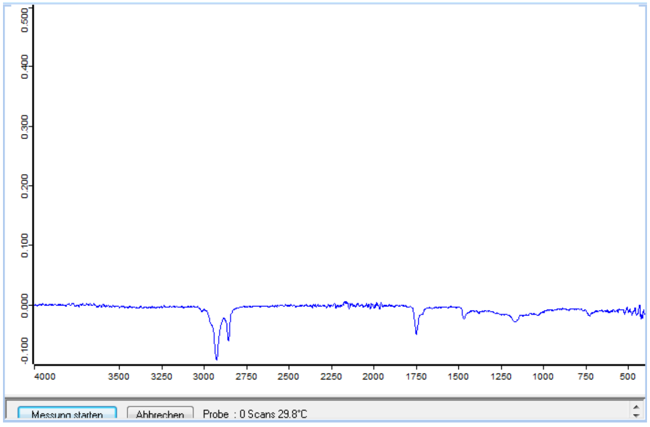
After having cleaned the ATR crystal, you can check it for cleanliness using the live preview in OPUS. Proceed as follows:

1. Make sure that the anvil is not pressed against the ATR crystal.
2. Select in the *Measure* menu the *Advanced Measurement* function.
3. Measure the background spectrum by clicking on the *Background Single Channel* button.
4. Clean the ATR crystal once again.

➢ Note: For the live preview, the *Display single scans before measurement* check box on the *Display* dialog page needs to be activated. This is the default setting.

5. Measure the sample spectrum by clicking on the *Sample Single Channel* button.

➢ Thereupon, the live preview spectrum is displayed. From this spectrum, you can draw conclusions about the cleanliness of the ATR crystal.

 Probe : 0 Scans 29.9°C	A straight baseline in the preview is an indication of a clean ATR crystal which is (almost nearly) free of any sample residues. In this case, you can continue with the next sample measurement.
 Probe : 0 Scans 29.8°C	Negative bands in the live preview spectrum are an indication of sample residues on the ATR crystal during the background measurement. In this case, repeat the whole procedure (i.e. 1. cleaning, 2. background measurement, 3. cleaning 4. sample measurement) until a straight line is displayed in the preview.

5.12.9 Exchanging the ATR crystal plate

General information

Only in case of the non-heatable variant (not high-pressure), the ATR crystal plate can be exchanged. The following ATR crystal plates are available:

- plate with diamond ATR crystal
- plate with germanium ATR crystal

ATR Crystal material	**Color**	**Spectral range [cm^{-1}]**	**Refraction index**
Diamond	transparent	7,500 - 350	n = 2.43
Germanium	silver gray	5,000 - 550	n = 4.01

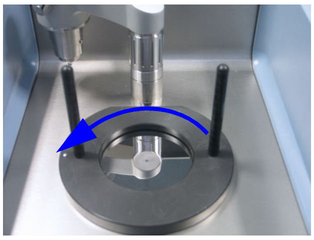
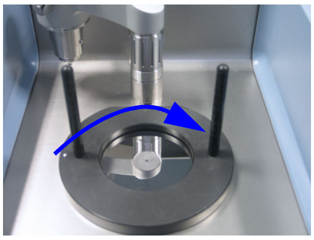
ATR Crystal material	**Suited for**
Diamond	all kinds of sample material, especially for hard and sharp-edged samples
Germanium	samples with a high absorptivity, especially for carbon-filled samples (e.g. O-rings, polymers)

Required tools

The required tools are included in the delivery scope of the ATR unit.

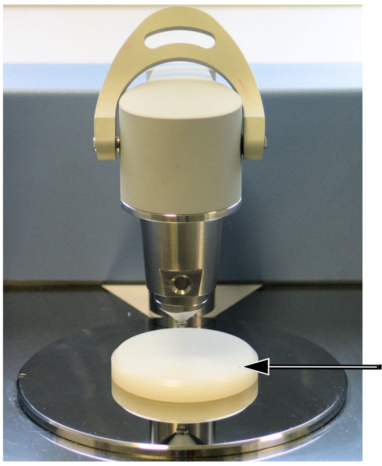
	Special tool for removing / installing the ATR crystal plate
	Suction cup

Procedure

	1. Pivot the pressure application device out of the measurement position.
	2. Put the special tool on the ATR crystal plate with the flat pointing to the rear. 3. Grasp the tool at the two handles and rotate it counter-clockwise until the ATR crystal plate is unscrewed. 4. Then, remove the tool.
	5. Put the suction cup in the ATR crystal plate and lift up the plate.
	6. Position the other crystal plate onto the ATR unit and put the special tool on the ATR crystal plate with the flat pointing to the rear. 7. To tighten the crystal plate, rotate it clockwise. as far as it goes.

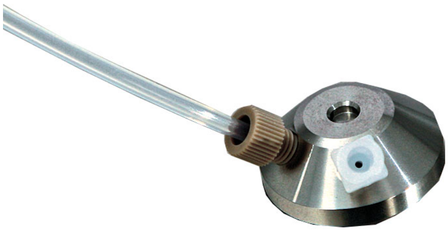
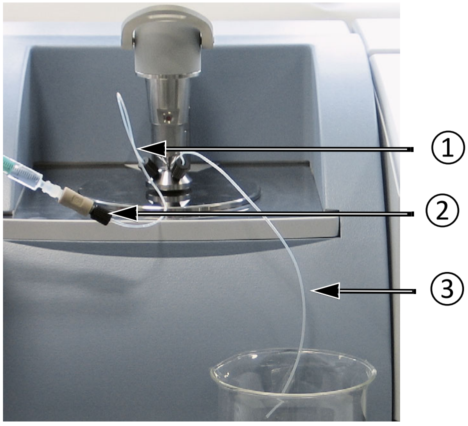
5.12.10 Optional components

5.12.10.1 Cover for volatile liquids

	① - Cover for volatile liquids When you measure volatile liquids, it is advisable to use this special cover. Apply the sample liquid on the ATR crystal and put the cover over it. Note: There is no need of applying a pressure on the cover.

5.12.10.2 Flow-through attachment for the ATR unit

General information

	The flow-through attachment is intended for the analysis of liquids with a ATR unit in flow-through or stopped-flow-mode. With this accessory, the change of concentration due to evaporation will be prevented effectively. Sample liquids can be easily injected with a syringe or an auto sampler. You can also connect a pump which pumps the sample liquid continuously in the flow-through attachment.
	The flow-through attachment has two openings. Via one opening, the liquid enters the cell, via the other opening the liquid exits the flow-through attachment again. At each opening, a hose is connected. Note: The filling hose ① has an injection port for the Luer syringe ②, whereas the drainage hose ③ does not have such a port. Route the drain hose into a vessel for recollecting the exiting liquid.

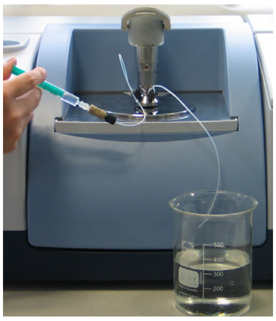
Specifications

Parameter	Specification
Materials	Body: Stainless steel O-ring: VITON Fittings: PEEK Luer-adapter: ETFE Connections: 10" Teflon PTFE-tubing (1/8"OD, 1.55mm ID)
Volume	30µm
Pressure	max. 7 bar

Fixing the flow-through attachment

	Place the flow-through attachment ① on the ATR crystal and fix the flow-through attachment by lowering the pressure application device. **Attention:** To ensure that the opening at the flow-through attachment bottom side is above the ATR crystal, position the flow-through attachment in such way that the anvil snaps into the indentation at the flow-through attachment top side when you press the anvil down. Note: If the flow-through attachment does not fit between ATR crystal and anvil you have to increase the height of the pressure application device first. ☞ See section 5.12.3.2.

Filling the flow-through attachment with a liquid sample

	1. Draw up sample liquid into the Luer syringe. 2. Insert the Luer syringe in the injection port at the filling hose. 3. Inject the liquid.

Cleaning the flow-through attachment

Clean the flow-through attachment, the ATR crystal surface and the complete sample contact surface thoroughly before you fill a new sample liquid into the attachment. Otherwise, residues of the previous sample liquid can falsify the measurement result.

☞ For detailed information about how to clean the ATR crystal plate, see section 5.12.7.

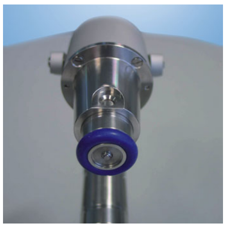
For cleaning the flow-through attachment, the following cleaning agents are suitable:

- Ethanol
- Isopropanol
- Water

Proceed as follows:

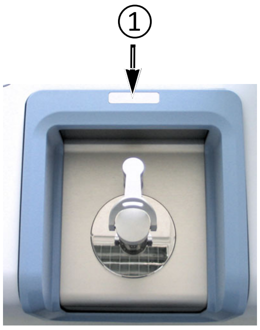
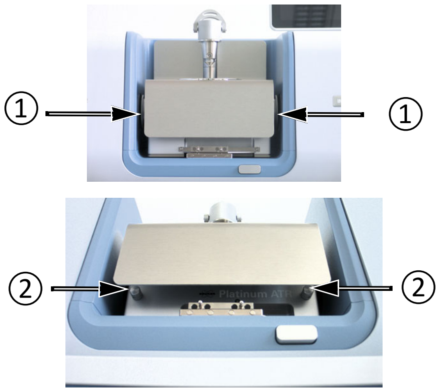
1. Flush the flow-through attachment thoroughly with an adequate cleaning agent and / or water. (Note: The appropriateness of a cleaning agent depends on the liquid you have analyzed before.)
2. Afterwards, purge the flow-through attachment with dry air until the interior of the cell is dry.

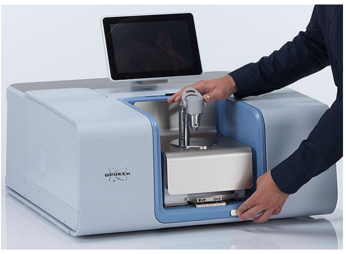
5.12.10.3 Attachment for ATR anvil die

 	This optional screw-on type attachment for the anvil is intended for measuring reaction-sensitive samples under inert condition. Moreover, it is suitable for measuring fine-powdered samples. To mount the optional attachment for the ATR anvil die, proceed as follows: 1. First remove the standard anvil by unscrewing it. 2. Then screw on the optional attachment for the ATR anvil die.

5.12.11 Removing / reinstalling the integrated ATR unit

Note: Basically, the integrated ATR unit is not intended for being removed from the sample compartment. If, however, a removal is necessary for good reason, proceed as follows.

1		Remove the metallic plate ①. Note: The plate is held by magnets.
2		Loosen the two Allen screws ② using a Allen wrench (size 3 mm).
3		Remove the blue cover frame.
4		Retract the two telescopic arms ① - one telescopic arm at the left side and one telescopic arm at the right side of the ATR unit - by turning the two knurled knobs ②. Note: The knurled knobs are behind the covering panel. Turn the left knurled knob clockwise and the right knurled knob counter-clockwise.

5		Press the QuickLock button to unlock the ATR unit.
6		Take the accessory out of the QuickLock mechanism in the sample compartment. Be careful not to damage the contact strips.
7		Press the QuickLock button.
8		Install the sample compartment cover by pressing the release button and inserting the pins at the cover in the corresponding holes.

To reinstall the ATR unit, proceed as follows:

1. Remove the sample compartment cover, if installed.
2. Place the ATR unit in the sample compartment and lock it with the QuickLock mechanism. See section 5.4.2.
3. Extend the two telescopic arms using the knurled knobs. (Note: Turn the left knurled knob counter-clockwise and the right knurled knob clockwise.)
4. Fit in the covering frame and fasten it with the two Allen screws. Put the metallic plate into the recess. (Note: The plate is held by magnets.)

6 Repair and Maintenance

6.1 General information

The spectrometer is a low-maintenance instrument.

The following maintenance and repair works can be performed by the user:

- Replacing the desiccant cartridge and regenerating the desiccant
- Restoring the dewar vacuum of a liquid nitrogen-cooled detector
- Replacing a damaged sample compartment window
- Cleaning the spectrometer

Perform only those maintenance and repair works which are described in this manual. Adhere strictly to the described procedures and observe all relevant safety precautions. Otherwise, personal injury and/or spectrometer damage can be the result. In this case, Bruker does not assume any liability. Maintenance and repair works which are not described in this manual have to be performed by Bruker service personnel only. For the Bruker service contact data, see section 1.6.

NOTE

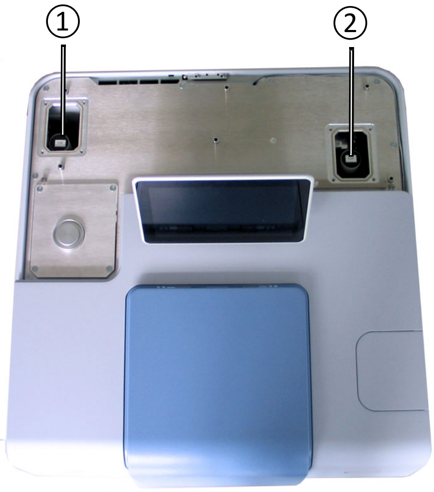
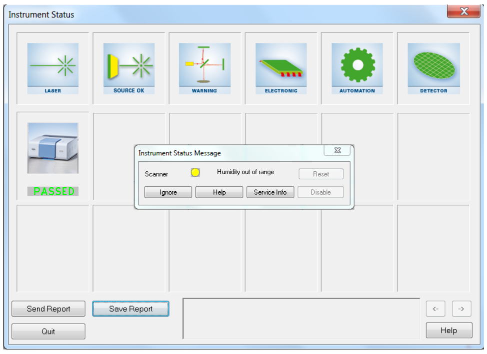
Damage to ESD-sensitive electronic spectrometer components because of accidental electrostatic discharges (ESD)

➢ Make sure that you are electrostatically discharged before you touch any electronic spectrometer component. Either use a grounded wrist strap or touch a grounded object (e.g. radiator). Note: The grounded wrist strap is the most effective (and the preferred) grounding method.

6.2 Replacing the cartridge and regenerating the desiccant

6.2.1 General information

The desiccant (molecular sieve) is in a cartridge. The molecular sieve adsorbs the water vapor of the ambient air. A saturated molecular sieve can be regenerated repeatedly by heating.

	The spectrometer is equipped with two desiccant cartridges: ① and ②. Both desiccant cartridges are situated in the optical bench compartment.
 Scanner Humidity out of range	The desiccant cartridges should be replaced approximately every six months or at least when the instrument status message *Humidity out of range* is displayed in OPUS.

You can either regenerate the desiccant as described in section 6.2.4 and reuse it or order a new desiccant cartridge. (For the order number refer to section B.1.)

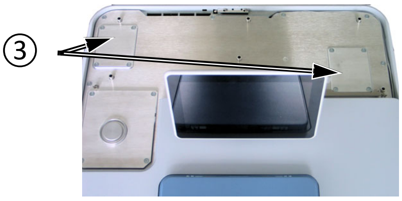
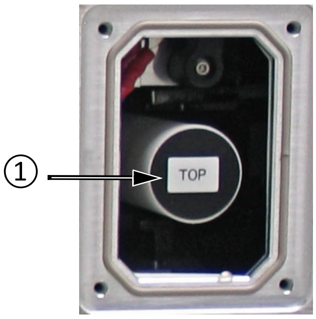
6.2.2 Storage notes

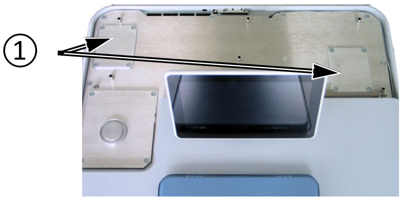
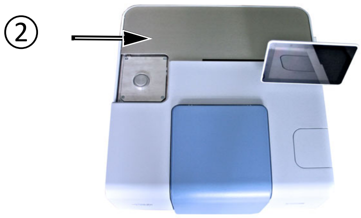
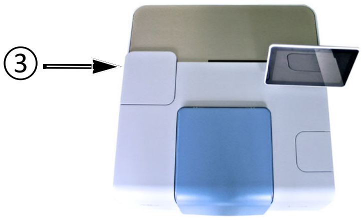
To maintain the serviceableness of the desiccant during the storage period, **store a new or regenerated cartridge always in a dry environment**!

Store a regenerated desiccant cartridge in a dry environment (e.g. in an desiccator or in an dry and airtight sealed container) until it is reused in the spectrometer.

6.2.3 Replacing the desiccant cartridges

	**Required tool** • TORX screw driver Note: This tool is included in the delivery scope.

1		**To gain access to the desiccant cartridges:** 1. Remove the plastic cover ① which provides access to the DigiTect detector. Note: This cover is held in place magnetically.
		2. Remove the metallic cover ②.
		3. Remove the two lids ③ which provide access to the desiccant cartridges by loosening the four TORX screws ④ at each lid. ☞ Note: In case the spectrometer is equipped with a touch panel, position the touch panel in such a way that you get easy access to the desiccant cartridge. For information about positioning possibilities of the touch panel, see section 4.2.
2		**To replace the desiccant cartridge:** Pull the desiccant cartridge ① out of the holder. Insert a new or regenerated desiccant cartridge into the holder. Ensure that the cartridge top side (with the label TOP) is upturned.

3		**To close the spectrometer:** 1. Reinstall the two lids ① and fasten the four screws at each lid.
		2. Put the metallic cover ② back in place. Note: The cover is held in place magnetically. Ensure that it is positioned correctly.
		3. Put the plastic cover ③ back in place. Note: This cover is held in place magnetically. Ensure that it is positioned correctly.

6.2.4 Regenerating the desiccant

A desiccant saturated with moisture can be regenerated repeatedly by heating up.

Safety notes

When regenerating the desiccant, observe the following safety notes:

CAUTION

Health hazard because of improper handling of the desiccant

Non-observance of the following safety instructions could result in minor health problems.

- ➢ Avoid skin and eye contact. Direct contact with the desiccant may cause minor skin and eye irritations. To avoid skin contact it is highly recommended to wear rubber gloves when handling with the desiccant.
- ➢ Avoid generating dust. The desiccant might be harmful if inhaled.
- ➢ Observe also the safety and handling instructions of the attached safety data sheet.

Procedure

1. Pull off the cap from the cartridge top side. (Note: This cap is labeled TOP.)
2. Empty the desiccant (molecular sieve) into a container that can withstand high temperatures (at least 150 °C).
3. Put the container in an oven for at least 24 hours at a temperature of 150°C. **ATTENTION: Do not heat the desiccant over 160°C!**
4. Refill the regenerated desiccant in the cartridge and close the cartridge again with the cap.
5. Store the regenerated desiccant cartridge in a dry environment (e.g. in an desiccator or in an dry and airtight sealed container) until it is reused in the spectrometer. (Note: A dry storage location will maintain serviceableness of the regenerated desiccant during the storage period.)

6.3 Restoring the dewar vacuum of a liquid nitrogen-cooled detector

6.3.1 General information

The operating temperature of a liquid nitrogen-cooled detector (e.g. MCT detector) is significantly below room temperature. To achieve the required operating temperature, these detectors are cooled down with liquid nitrogen. The available liquid nitrogen-cooled detector detectors have different nominal hold times[1]: 8, 12 or 24 hours. To provide for the longest possible hold time, the detector is integrated in a dewar. So, the actual hold time strongly depends on the quality of the vacuum in the detector dewar.

If the actual hold time decreases considerably with regard to the nominal hold time, the detector dewar vacuum needs to be restored. The existence of condensation water on the detector outside indicates that the vacuum must be restored soon. Another indication that a vacuum restoration is required is a failed *Ice Band Test*[2]. If the detector outside is iced the detector dewar vacuum must be restored immediately. For evacuating the dewar, the detector must be removed from the spectrometer.

6.3.2 Evacuating the detector dewar

Required evacuating equipment

- Vacuum pump (turbo molecular pump or oil-free high-vacuum pump that is capable of generating a vacuum of at least < 10^{-5} mbar)
- Adapter for connecting the vacuum pump to the detector dewar
- Shut-off valve
- 2x flexible metal hoses

i The above listed evacuating equipment is NOT included in the standard delivery scope of the liquid nitrogen-cooled detector. If desired, Bruker offers suitable evacuating equipment (part number S105-V2, D126 and I10290). Alternatively, Bruker also offers the service of evacuating the detector dewar (part number SD128). This option requires the removal of the liquid nitrogen-cooled detector from the spectrometer and the sending of the complete detector to Bruker for evacuation.

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[1] The hold time indicates how long the cooling effect of the liquid nitrogen lasts.

[2] The *Ice Band Test* checks whether there is a thin ice layer on the detector element. This in turn is an indication of the vacuum quality in the detector dewar. The *Ice Band Test* is part of the PQ test protocol. For detailed information, refer to the OPUS Reference Manual.

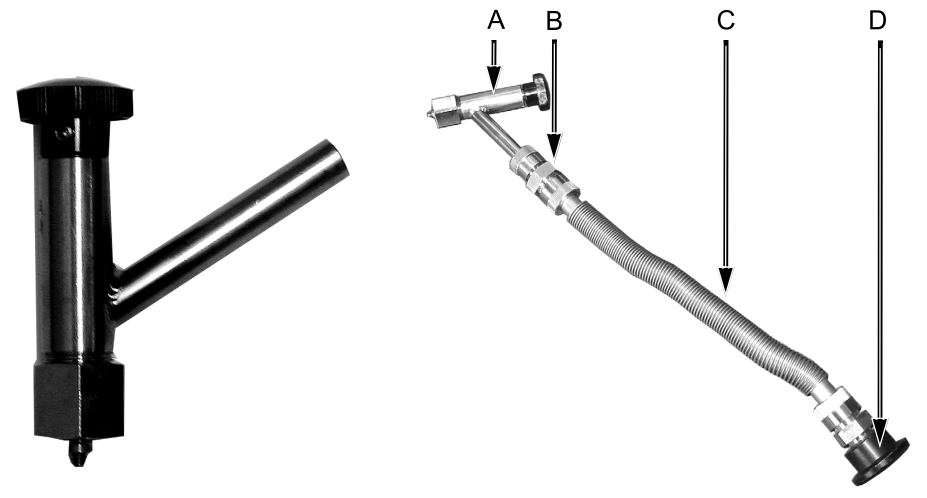

Figure 6.1: a) Adapter b) Adapter with flexible Metal Hose and Flange

Fig. 6.1	Component
A	Connecting adapter (for connecting the vacuum pump to the detector dewar)
B	Flange
C	Flexible metal hose
D	NW 25 flange (for connecting to the vacuum pump)

Procedure

➣ Before starting to evacuate the detector dewar, make sure that the dewar does not contain any more liquid nitrogen and that the detector has warmed up to room temperature. Take into consideration that the detector warming-up from operating temperature to room temperature takes at least 3 hours after the residual liquid nitrogen has been emptied.

1. Remove the detector from the spectrometer. See section 5.9.2.
2. Connect the adapter to the vacuum pump by flanging a flexible metal hose to the connecting piece of the adapter (E in fig. 6.3) and to the vacuum pump. See fig. 6.1b. (Note: The connecting piece of the adapter has an OD of 9.7mm.) In addition, install a shut-off valve between adapter and vacuum pump.
3. Make sure whether the shut-off valve is closed. Switch on the vacuum pump. Leave the pump running until it has reached its operating temperature.
4. Inspect the O-ring inside the adapter (C in fig. 6.3) for signs of wear.

➣ The O-ring inside the adapter is a wearing part that needs to be replaced after 4 or 5 evacuations at maximum.

5. Remove the cap from the connection nozzle of the detector. (See fig. 6.2a.)

6. Pull the adapter knob (G in fig. 6.3) to the open position and loosen the coupling nut (A in fig. 6.3).
7. Push the adapter carefully over the connection nozzle of detector dewar and fasten the coupling nut (A in fig. 6.3 hand-tight while holding the adapter and the detector as shown in fig. 6.2b. (A hand-tight tightening of the coupling nut is sufficient.)

➢ Hold the adapter and the detector always as shown in fig. 6.2b when you have to carry out the following tasks: opening and closing the evacuation valve by pushing or pulling the adapter knob (step 8, 12, 14 and 17), screwing the threaded adapter rod in or out of the connection thread of the dewar evacuation valve (step 11 and 15) and loosening the coupling nut (step 18).

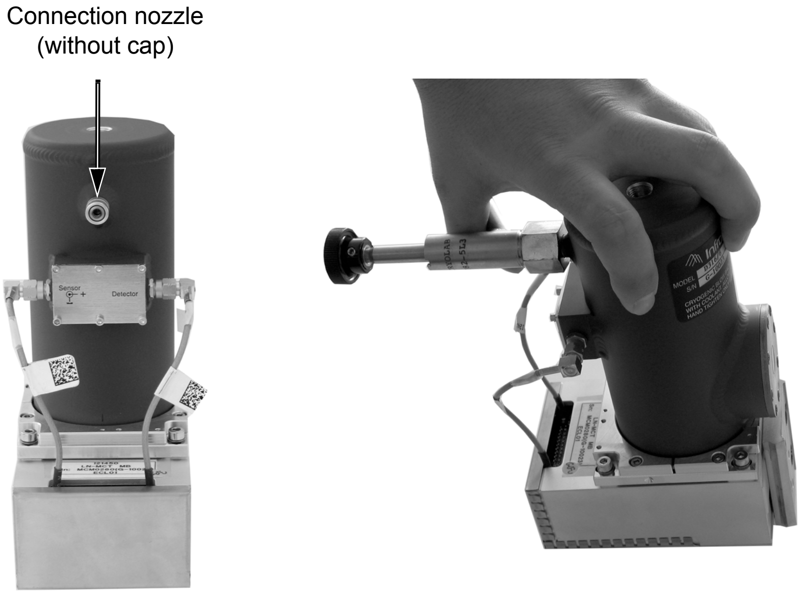

Figure 6.2: a) MCT detector

b) How to hold the MCT detector when opening or closing the dewar evacuation valve

8. Push the adapter knob (G in fig. 6.3) in the closed position until the threaded rod (D in fig. 6.3) of the adapter is in contact with the sealing plug of the dewar evacuation valve.
9. Before you begin to evacuate the detector dewar, check the connections for leak tightness by evacuating the section between vacuum pump and detector at first. To do this, open the shut-off valve. If a vacuum of 10^{-4}mbar is generated within a few minutes it is an indication of the leak tightness of this section.
10. Close the shut-off valve again.
11. Screw the threaded rod of the adapter (D in fig. 6.3) in the connection thread of dewar evacuation valve by turning the adapter knob (G in fig. 6.3) clockwise; 2 to 3 rotations are sufficient. **Attention: In case of more than 2 or 3 knob rotations there is a risk that the threaded connection becomes inseparable! That means the threaded rod of the adapter cannot be screwed out of the connection thread of the dewar evacuation valve again.**
12. Pull the knob (G in fig. 6.3) to the open position in order to open the dewar evacuation valve.
13. Begin to evacuate the detector dewar by opening the shut-off valve.

➢ We recommend an evacuation time of at least 3 days to allow for generating an optimal vacuum inside the dewar. The final pressure in the detector dewar should be less than 10^{-5} mbar.

14. When the optimal vacuum is achieved, close the dewar evacuation valve by pushing the adapter knob (G in fig. 6.3) to the closed position. Press the adapter knob firmly to the stop position to ensure that the dewar evacuation valve is sealed airtight.
15. Screw the threaded rod of the adapter (D in fig. 6.3) out of the connection thread of the dewar evacuation valve by rotating the adapter knob (G in fig. 6.3) several turns counterclockwise until you sense that the threaded adapter rod and the connection thread of the dewar evacuation valve are not joint any more. Be careful in order to prevent an unintentional opening of the evacuation valve and consequently to prevent the detector dewar from being vented again.
16. Vent the section between vacuum pump and adapter.
17. Pull the knob (G in fig. 6.3) to the open position. Attention: Make sure that the sealing plug of the evacuation valve is NOT pulled out! This may occur when you have screwed the threaded adapter rod too far in the connection thread of the dewar evacuation valve. (See step 10.) In this case repeat the dewar evacuation. If you do not succeed in closing the evacuation valve at all, you have to send the detector to Bruker.
18. Loosen the coupling nut (A in fig. 6.3) and remove the adapter from the connection nozzle of the detector dewar.
19. Reinstall the detector in the spectrometer. See section 5.9.2.

➢ If a tiny amount of air should unawares get into the detector dewar during the evacuation procedure (e.g. when you close the evacuation valve) you can perform measurements with this detector for the moment but after a relatively short period of time you have to repeat the detector evacuation.

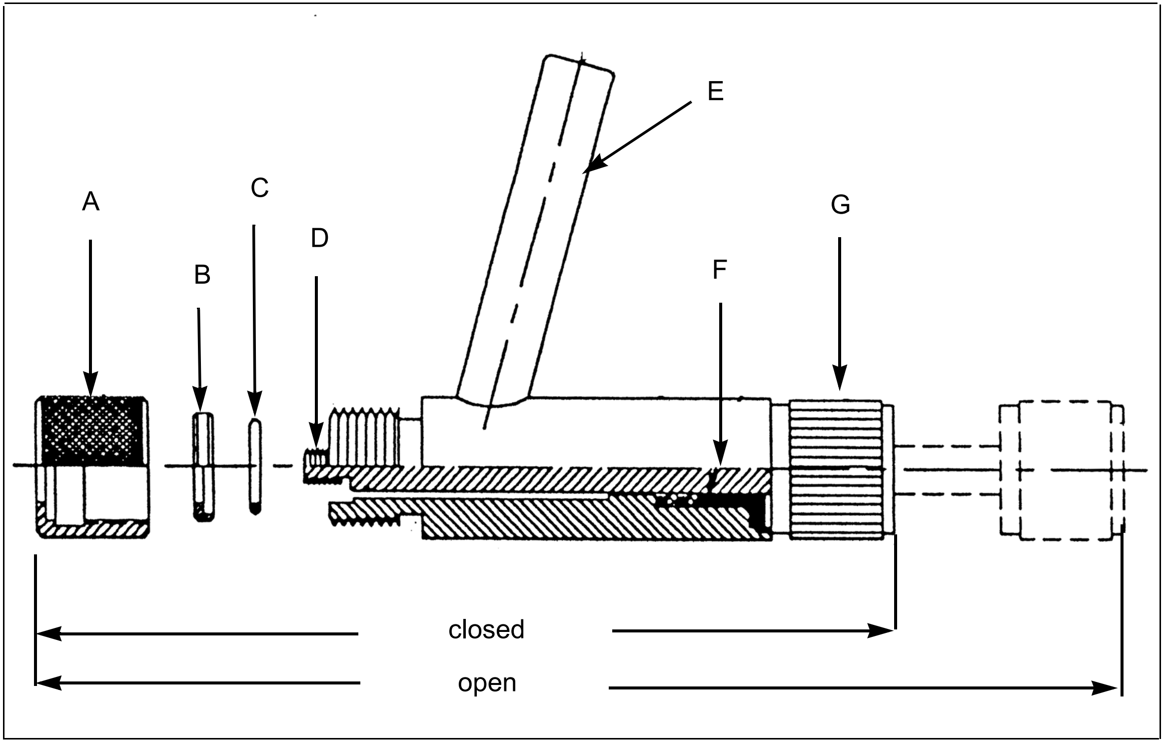

Figure 6.3: Connecting adapter - Cross section

Fig. 6.3	Components of the connecting adapter
A	Coupling nut
B	O-ring retainer
C	O-ring
D	Threaded rod (to remove the valve closure of the detector dewar)
E	Connecting piece for vacuum pump (OD = 9,7mm)
F	Washer and O-ring packing
G	Knob

6.4 Replacing a broken or opaque sample compartment window

6.4.1 General information

A sample compartment window needs to replaced only if it is broken, dirty or opaque and the opaqueness has reached such a degree that the transparency (infrared transmittance) is seriously reduced.[1]

The sample compartment windows are held by magnets. The window assembly is electronically coded with an ID chip.

☞ For the order number of the sample compartment windows, refer to section B.2.

6.4.2 Handling instruction

NOTE

Irreversibly damaged sample compartment window because of improper handling

The sample compartment window is a delicate component. Observe the following handling instructions to ensure a long service life.

➢ The window is very fragile. Handle it with care because it can crack easily. Avoid any mechanical impact.

➢ Do not touch the window surface. This may lead to irreversible contamination. (Note: Contaminations on the window surface can decrease the IR-transparency significantly.)

➢ Do not try to clean a window. This will lead to irreversible damages.

➢ Most of the window materials are hygroscopic. Store them under dry conditions.

6.4.3 Safety note

Some sample compartment windows are of a material which is harmful or (very) toxic. (See section 4.5.5.) During normal spectrometer operation, these materials do not pose any health hazard. However, if such a window should break because of mechanical impact, be extremely careful.

⚠ WARNING

Health hazard because of improper handling of broken harmful or toxic window material

Non-observance of the following safety instructions could result in death or serious injury.

➢ Avoid generating dust of broken window material. This material is harmful or toxic if swallowed or inhaled.

➢ Also avoid skin and eye contact.

➢ Dispose the harmful or toxic material according to the laboratory regulations and the national regulations.

➢ Observe also the safety and handling instructions given in the safety data sheet for the material in question.

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[1] Especially windows made of hygroscopic material tend to become opaque in the course of time. For an overview of the available window materials and their properties, see section 4.5.5.

6.4.4 Replacement procedure

	**Required tool** Special tool for removing / installing a window or flange Note: This tool is included in the delivery scope of the spectrometer.

1		Open the large-sized sample compartment.
2		**Remove the window assembly:** Position the tool with the label TOP pointing upwards.
		Insert the pins of the tool into the corresponding holes of the window assembly. Note: The tool is attracted magnetically to the window assembly.
		Slightly rotate the tool to overcome the magnetic attractive force.
3		**Reinstall the window assembly:** Insert the pins of the tool into the corresponding holes of the window assembly. Position the tool with the label TOP pointing upwards and attach it to the sample compartment wall in such a way that the electronic contacts at the window assembly and the electronic contacts at the sample compartment wall have contact with each other. The window assembly is attracted magnetically to the sample compartment wall. ➣ A beep indicates that the window has been recognized by the electronics.

6.5 Performing an OQ test[1] with OVP[2]

After the replacement of a defective optical component[3], it is highly recommended to perform an OQ test for the test channels in question to ensure that the spectrometer achieves the specified parameter values[4].

Whenever accessories are used, it is essential to check the performance of the spectrometer with installed accessory in addition to the performance of the spectrometer itself. A misaligned accessory, for example, can strongly influence the performance of the analysis system even if the performance of spectrometer itself is OK.

Important Note: The resolution test, which is part of the OQ test protocol, requires a gas cell filled with carbon monoxide at low pressure If you do not have such a gas cell at your disposal, contact the Bruker service. For the Bruker service contact data, see section 1.6. Alternatively, you can disable this test of the OQ test protocol.

6.6 Cleaning the spectrometer

If required, you can clean the outer spectrometer housing with a dry or damp cloth.

NOTE

Spectrometer damage because of improper cleaning

➢ Do not use detergents with organic solvents, acids or bases!

➢ Do not clean the spectrometer interior. This may lead to serious spectrometer damage.

➢ Do not rub dirt or dust particles off a mirror surface, not even with a lens cloth or a lens tissue! Otherwise, the mirror will be damaged irreversibly. Blow off dust particles on the mirror surface using compressed air, for example. In case you do not succeed in blowing off the dirt, contact the Bruker service. (See section 1.6.)

---

[1] OQ test - Operational Qualification Test

[2] OVP - OPUS Validation Program (It is intended for performing spectrometer validation tests like OQ and PQ.)

[3] Perform the OQ test only after the replacement of a defective component, but NOT after exchanging an optical component for the purpose of extending the spectral range, for example.

[4] In the course of the OQ test, the following parameters are tested: resolution, sensitivity, energy distribution, wavenumber accuracy, photometric accuracy, scan time, peak position and peak amplitude.

7 Troubleshooting

7.1 General information

This chapter deals mainly with the most common spectrometer problems that may occur as experience has shown. It provides information about possible causes of the problem and presents solutions for troubleshooting. If the solutions listed in this chapter do not eliminate your spectrometer fault contact the Bruker service.

☞ For the Bruker service contact data refer to section 1.6.

Depending on how a spectrometer problem becomes apparent, they are divided in the following categories:

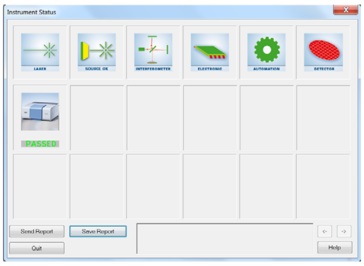
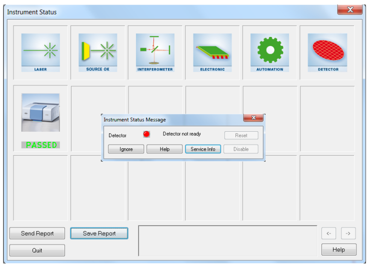
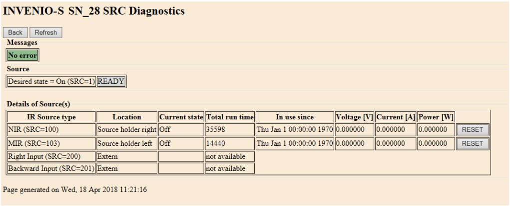
- Spectrometer problem indicated by status indicator (LED strip below the large-sized sample compartment)
- Spectrometer problem indicated by an instrument status message in OPUS
- No communication between spectrometer and computer
- A signal check in OPUS reveals that no signal is detected or that the signal intensity is too low.
- A failed validation test (e.g. PQ test)

The available diagnostic means (e.g. spectrometer status indicator LED, instrument status messages in OPUS, diagnostics pages of the spectrometer firmware) enable the operator to identify many spectrometer problems, or at least to narrow down a problem.

☞ The available diagnostic means are described in detail in section 7.2. In addition, there is the possibility of a remote fault diagnosis by the Bruker service. See section 7.4.

7.2 Diagnostic means

For a spectrometer fault diagnosis, the following diagnostic means are at your disposal:

<table>
<tr>
<td> </td>
<td>Spectrometer status indicator (LED strip ① below the large-sized sample compartment
☞ See section 7.2.1</td>
</tr>
<tr>
<td> </td>
<td>OPUS dialog window <i>Instrument Status</i>
☞ See section 7.2.2.</td>
</tr>
<tr>
<td>
Detector ● Detector not ready</td>
<td>Instrument status messages in OPUS
☞ See section 7.2.3.</td>
</tr>
<tr>
<td>
INVENIO-S SN_28 SRC Diagnostics

Messages
No error
Source
Desired state = On (SRC=1) READY
Details of Source(s)
<table>
<tr><th>IR Source type</th><th>Location</th><th>Current state</th><th>Total run time</th><th>In use since</th><th>Voltage [V]</th><th>Current [A]</th><th>Power [W]</th><th></th></tr>
<tr><td>NIR (SRC=100)</td><td>Source holder right</td><td>Off</td><td>35598</td><td>Thu Jan 1 00:00:00 1970</td><td>0.000000</td><td>0.000000</td><td>0.000000</td><td>RESET</td></tr>
<tr><td>MIR (SRC=103)</td><td>Source holder left</td><td>Off</td><td>14440</td><td>Thu Jan 1 00:00:00 1970</td><td>0.000000</td><td>0.000000</td><td>0.000000</td><td>RESET</td></tr>
<tr><td>Right Input (SRC=200)</td><td>Extern</td><td></td><td>not available</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>Backward Input (SRC=201)</td><td>Extern</td><td></td><td>not available</td><td></td><td></td><td></td><td></td><td></td></tr>
</table>
Page generated on Wed, 18 Apr 2018 11:21:16</td>
<td>Diagnostics pages of the spectrometer firmware
☞ See section 7.2.4.</td>
</tr>
</table>

7.2.1 Spectrometer status indicator

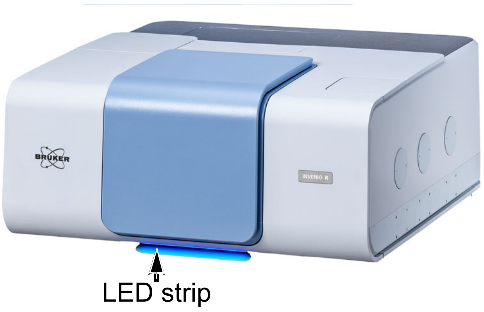


Figure 7.1: Location of the spectrometer status indicator

Below the large sample compartment, there is a LED strip which indicates the current spectrometer status. The color of the LEDs give a general indication of the operating status of the spectrometer.

LEDs light up bluish.	The spectrometer is initializing. Note: The LEDs light up bluish only for the duration of spectrometer initialization.
LEDs light up blue.	Instrument is OK and ready for measurement. This is the case when: • all optical components (e.g. NIR source, laser) achieve their performance specification and • the OVP tests (OQ and PQ) of the currently selected measurement channel have passed and are still valid.
LEDs light up yellow.	A yellow instrument status indicates a warning. This is the case when: • the end of the specified lifetime of the source and/or laser is nearly reached or • the validity period of an OVP test (OQ and/or PQ) of the currently selected measurement channel is expired or • an OVP test (OQ and/or PQ) of the currently selected measurement channel has failed or • the water vapor concentration inside the spectrometer is too high, i.e. it exceeds the factory-set limit value. Note: In case of a yellow instrument status LED, measuring is still possible, but the reliability of the measurement results is not ensured. For this reason, it is highly recommended to diagnose the cause of the warning and to eliminate it. **Important note:** In case you work in a validated environment, you have to diagnose the cause of the warning and to eliminate it before continuing with the measurements. Otherwise, 21CFR part 11-compliant measurement results are not ensured. ☞ See section 7.5.2 for troubleshooting.
LEDs light up red.	A red instrument status LED indicates an error. For example, this is the case when: • an optical component (e.g. NIR source, laser) fails or does not achieve its performance specification Note: In case the instrument status LED lights red, measuring is not possible until the cause of the error is eliminated. ☞ See section 7.5.1 for troubleshooting.

7.2.2 OPUS dialog *Instrument Status*

The OPUS dialog window *Instrument Status* allows you to diagnose which spectrometer component has caused the failure or to find out whether an OVP test[1] has expired or failed. To perform a fault diagnosis, proceed as follows:

1. Either click on the OPUS status light or select in the OPUS *Measure* menu the *Optics Diagnostics* function. The following dialog window opens:

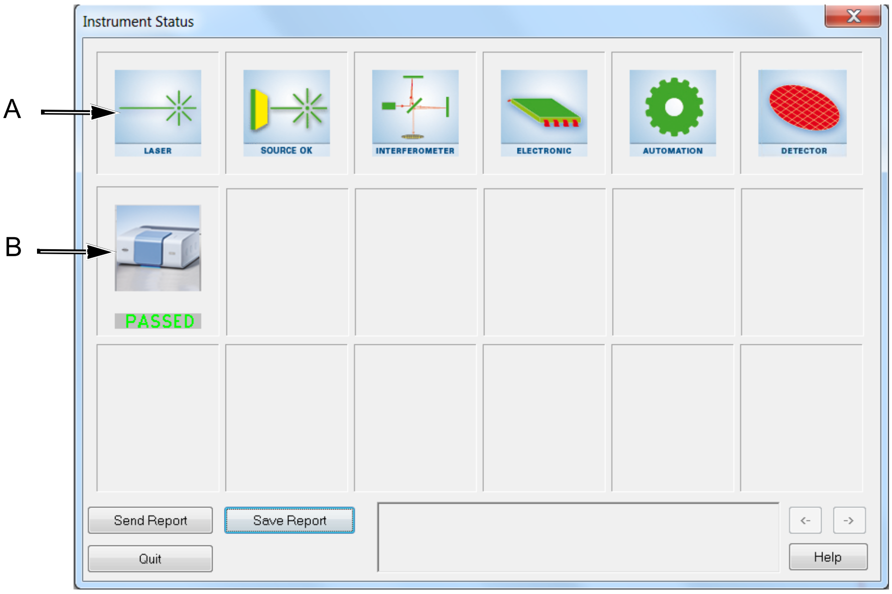
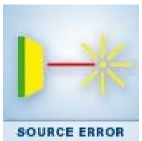


Figure 7.2: Optics Diagnostics - Instrument Status dialog

---

[1] "Validation test" is a collective term for all tests (e.g. OQ - Operational Qualification, PQ - Performance Qualification) that can be performed with OVP in order to validate the spectrometer. OVP (OPUS Validation Program) is part of OPUS. The general purpose of these validation tests is to check whether the spectrometer system achieves the specified performance or not. For information about OVP refer to the OPUS Reference Manual.

A) The status of the hardware components, e.g. source, laser, interferometer etc. is displayed in the upper icon line. The status can be as follows:

	**OK** Component is okay.
	**WARNING** The exact meaning of a warning depends on the component in question. For example, in case of the source, a warning means: • End of the specified lifetime of the component is nearly reached. In this case, measuring is still possible. Note: In case of a warning, measuring is still possible. However, it is highly recommended to diagnose the cause of the warning and to eliminate it.
	**ERROR** Component is defective. In case of an error, measuring is no longer possible.

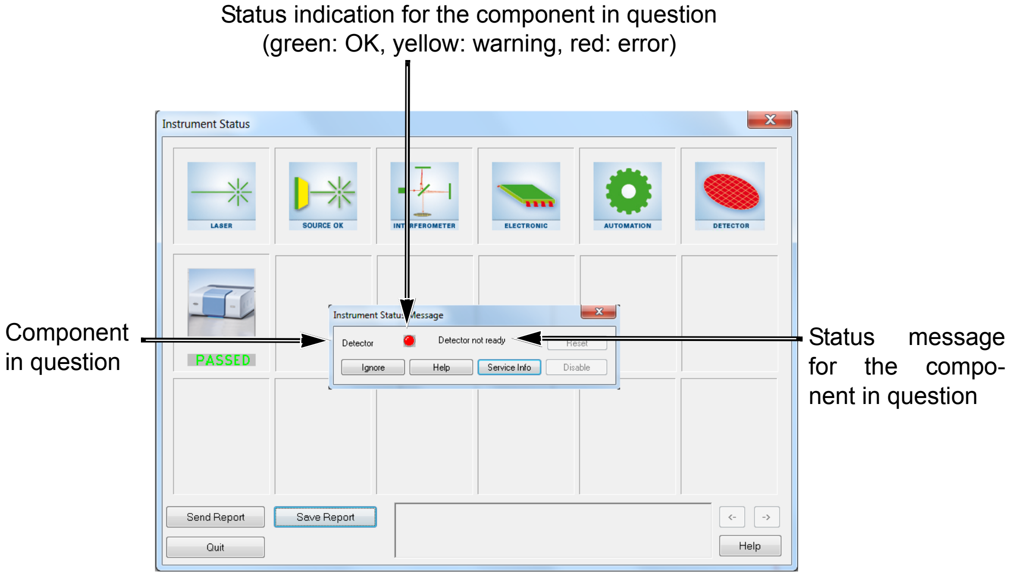
B) The second row of icons refers to the possible active test channels and indicates the result of the last OVP test performed. The results can be as follows:

	**PASSED (green):** OVP test passed. Test is still valid.
	**EXPIRED (light blue):** The validity period of an OVP test has expired. What to do in this case? Perform the OVP test in question. (See OPUS Reference Manual.)
	**FAILED (red):** OVP test failed. What to do in this case? Try to find out the cause of a failed OVP test by performing a systematic fault diagnosis. (See section 7.3 and section 7.5.5.) Solve the problem. Then repeat the OVP test in question.
	**INACTIVE (yellow):** This test channel has been set up but no OVP test has been performed yet and all OVP tests are disabled.

2. To perform a fault diagnosis of a particular spectrometer component click on the respective icon in the first row of the *Instrument Status* dialog. The *Instrument Status Message* dialog opens. (See fig. 7.3.)

7.2.3 Instrument status messages in OPUS

Some spectrometer problems are indicated additionally by a corresponding instrument status message displayed in OPUS. (See fig. 7.3.) These messages appear when you click on the icon of the optical component in question in the *Instrument Status* dialog.


Status indication for the component in question (green: OK, yellow: warning, red: error)

Component in question

Status message for the component in question

Instrument Status Message

Detector

Detector not ready

Figure 7.3: Instrument status message in OPUS indicating a scanner problem

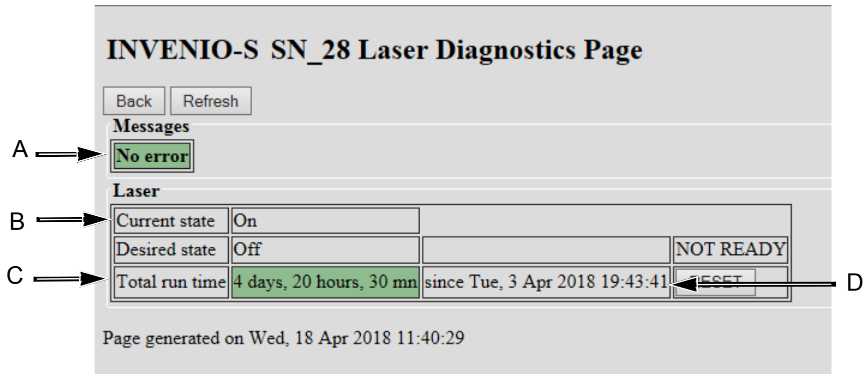
7.2.4 Diagnostic pages of the spectrometer firmware

When you click on the *Service Info* button (see fig. 7.3), the diagnostics page for the component in question opens. The diagnostics pages of the spectrometer firmware contain all relevant information about the current operating state of the respective spectrometer component. In the following figures, the information relevant to fault diagnostics are highlighted by a rectangle.

The following figures (fig.7.4 to fig. 7.9) show the diagnostics pages of the following spectrometer components:

- Laser (HeNe-Laser Diagnostics Page)
- Source (SCR Diagnostics)
- Interferometer (Scanner Diagnostics)
- Detector (DTC Diagnostics)
- Electronic (Instrument Ready Diagnostics)
- Automation (Automation units Diagnostics)

➢ The explanation of the diagnostic pages is restricted to the most important pieces of information which are relevant to the user for troubleshooting.



INVENIO-S SN_28 Laser Diagnostics Page

Messages

No error

Laser

Current state	On		
Desired state	Off		NOT READY
Total run time	4 days, 20 hours, 30 mn	since Tue, 3 Apr 2018 19:43:41	

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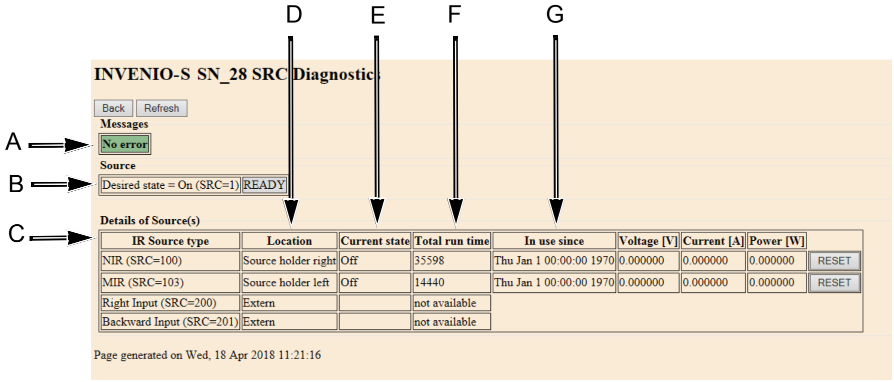
Figure 7.4: Laser diagnostics page

Fig. 7.4	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.
B	Current state: Current switch state of the laser Desired state: State selected by user
C	Total run time: Current reading of the laser operating hours counter
D	Date of putting the laser into operation for the first time



INVENIO-S SN_28 SRC Diagnostics

Messages

No error

Source

Desired state = On (SRC=1) READY

Details of Source(s)

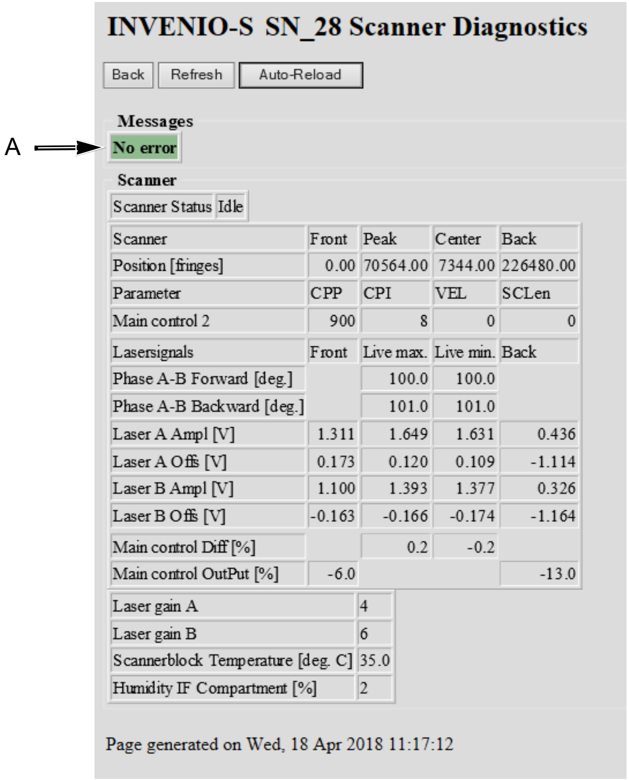
IR Source type	Location	Current state	Total run time	In use since	Voltage [V]	Current [A]	Power [W]	
NIR (SRC=100)	Source holder right	Off	35598	Thu Jan 1 00:00:00 1970	0.000000	0.000000	0.000000	RESET
MIR (SRC=103)	Source holder left	Off	14440	Thu Jan 1 00:00:00 1970	0.000000	0.000000	0.000000	RESET
Right Input (SRC=200)	Extern		not available					
Backward Input (SRC=201)	Extern		not available					

Page generated on Wed, 18 Apr 2018 11:21:16

Figure 7.5: Source diagnostics page

Fig. 7.5	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.
B	Desired state: State selected by user

Fig. 7.5	Explanation
C	IR source type: Currently installed source(s) are listed
D	Location: Installation location of the source(s)
E	Current state: Current switch state of the source(s)
F	Total run time: Current reading of the source operating hours counter(s)
G	In use since: Date of putting the source in question into operation for the first time



INVENIO-S SN_28 Scanner Diagnostics

Messages

No error

Scanner

Scanner Status	Idle

Scanner	Front	Peak	Center	Back
Position [fringes]	0.00	70564.00	7344.00	226480.00
Parameter	CPP	CPI	VEL	SCLen
Main control 2	900	8	0	0
Lasersignals	Front	Live max.	Live min.	Back
Phase A-B Forward [deg.]		100.0	100.0	
Phase A-B Backward [deg.]		101.0	101.0	
Laser A Ampl [V]	1.311	1.649	1.631	0.436
Laser A Offs [V]	0.173	0.120	0.109	-1.114
Laser B Ampl [V]	1.100	1.393	1.377	0.326
Laser B Offs [V]	-0.163	-0.166	-0.174	-1.164
Main control Diff [%]		0.2	-0.2	
Main control OutPut [%]	-6.0			-13.0

Laser gain A	4
Laser gain B	6
Scannerblock Temperature [deg. C]	35.0
Humidity IF Compartment [%]	2

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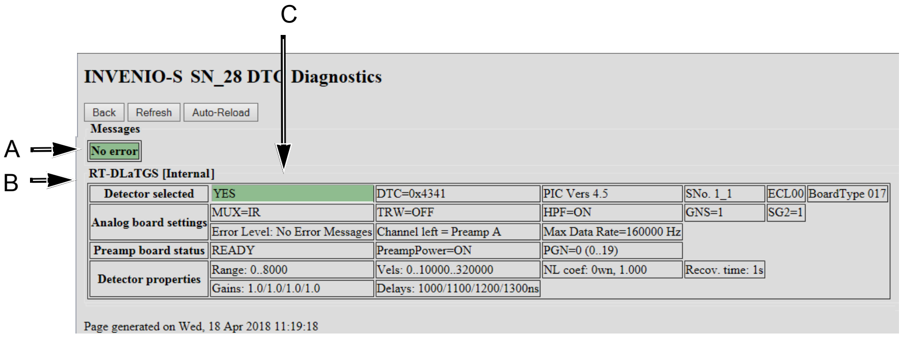
Figure 7.6: Scanner (Interferometer) diagnostics page

Fig. 7.6	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.



INVENIO-S SN_28 DTC Diagnostics

Messages

No error

RT-DLaTGS [Internal]

Detector selected	YES	DTC=0x4341	PIC Vers 4.5	SNo. 1_1	ECL00	BoardType 017
Analog board settings	MUX=IR	TRW=OFF	HPF=ON	GNS=1	SG2=1	
	Error Level: No Error Messages	Channel left = Preamp A	Max Data Rate=160000 Hz			
Preamp board status	READY	PreampPower=ON	PGN=0 (0..19)			
Detector properties	Range: 0..8000	Vels: 0..10000..320000	NL coef: 0wn, 1.000	Recov. time: 1s		
	Gains: 1.0/1.0/1.0/1.0	Delays: 1000/1100/1200/1300ns				

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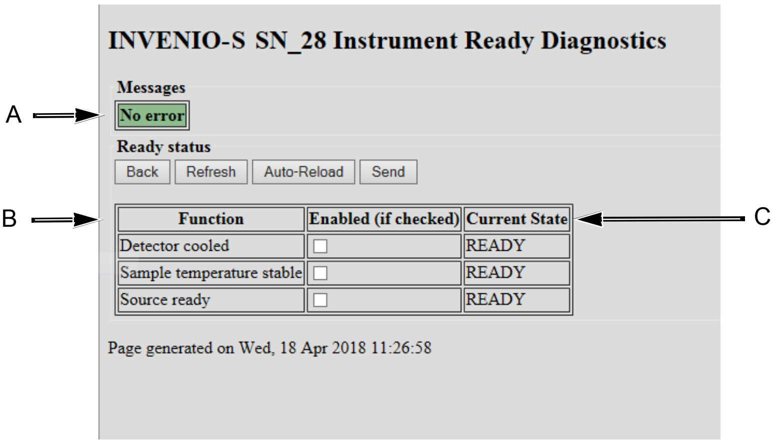
Figure 7.7: Detector diagnostics page

Fig. 7.7	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.
B	Installed detectors Note: The detector type (e.g. RT DLaTGS) and installation location (e.g. [Internal Pos.1]) are indicated.
C	Detector selected: (YES or NO): status of the current selection Note: The detector is selected in OPUS by the user.



INVENIO-S SN_28 Instrument Ready Diagnostics

Messages

No error

Ready status

Function	Enabled (if checked)	Current State
Detector cooled	☐	READY
Sample temperature stable	☐	READY
Source ready	☐	READY

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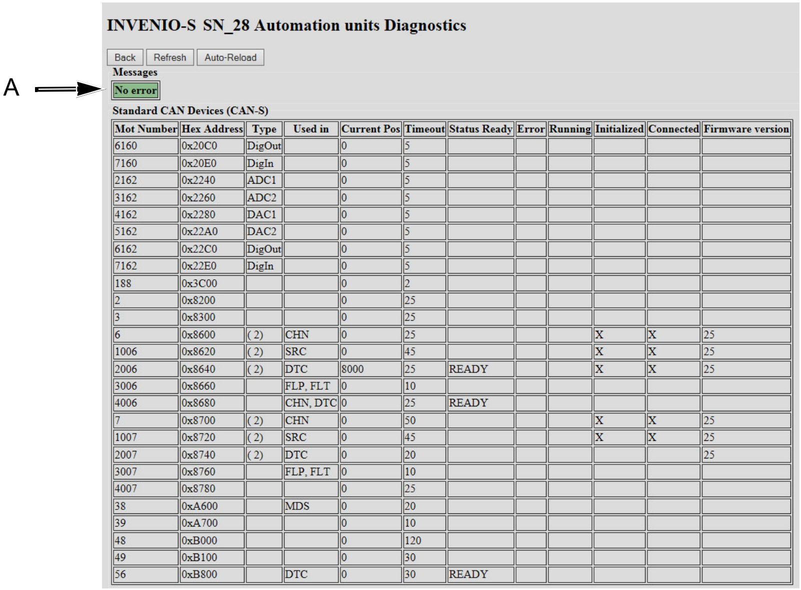
Figure 7.8: Electronics diagnostics page

Fig. 7.8	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.
B	Function: Parameters which define the readiness of the spectrometer to measure
C	Current state: Current switch state of readiness of the parameters in question



INVENIO-S SN_28 Automation units Diagnostics

Messages

No error

Standard CAN Devices (CAN-S)

Mot Number	Hex Address	Type	Used in	Current Pos	Timeout	Status Ready	Error	Running	Initialized	Connected	Firmware version
6160	0x20C0	DigOut		0	5						
7160	0x20E0	DigIn		0	5						
2162	0x2240	ADC1		0	5						
3162	0x2260	ADC2		0	5						
4162	0x2280	DAC1		0	5						
5162	0x22A0	DAC2		0	5						
6162	0x22C0	DigOut		0	5						
7162	0x22E0	DigIn		0	5						
188	0x3C00			0	2						
2	0x8200			0	25						
3	0x8300			0	25						
6	0x8600	(2)	CHN	0	25				X	X	25
1006	0x8620	(2)	SRC	0	45				X	X	25
2006	0x8640	(2)	DTC	8000	25	READY			X	X	25
3006	0x8660		FLP, FLT	0	10						
4006	0x8680		CHN, DTC	0	25	READY					
7	0x8700	(2)	CHN	0	50				X	X	25
1007	0x8720	(2)	SRC	0	45				X	X	25
2007	0x8740	(2)	DTC	0	20						25
3007	0x8760		FLP, FLT	0	10						
4007	0x8780			0	25						
38	0xA600		MDS	0	20						
39	0xA700			0	10						
48	0xB000			0	120						
49	0xB100			0	30						
56	0xB800		DTC	0	30	READY					

Figure 7.9: Automation units diagnostics page

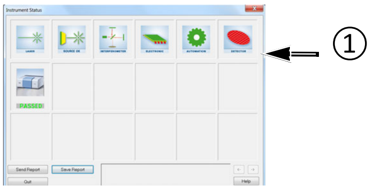
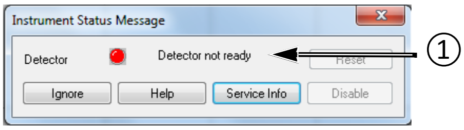
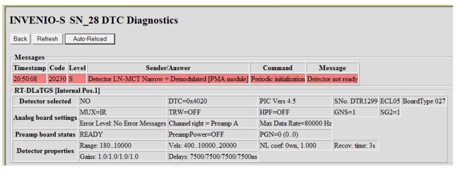
Fig. 7.9	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.

7.3 General information about how to diagnose a fault

In many cases, a problem caused by a spectrometer component, that is either defective or not properly installed or not in operating condition, becomes apparent in several different ways. For example:

- You have started a measurement but OPUS does not display any measurement result. (Reason: OPUS did not start the measurement at all because OPUS has recognized a spectrometer component error.)
- No signal detection or signal intensity is too low. (See section 5.10.)
- You have started a validation test but OVP does not display a PQ or OQ test protocol. (Reason: OVP did not start the validation test at all OPUS has recognized a spectrometer component error.)
- A failed OQ test or PQ test.

To find out the specific cause of a spectrometer problem, it is advisable to narrow down the trouble source in a systematic way. We recommend the following fault diagnosis procedure:

1		First check whether the spectrometer status indicator ① (LED strip below the sample compartment) or the status lamp ② in OPUS indicate a spectrometer problem. ➢ Are they red or yellow?
2		If so, open the OPUS dialog window *Instrument Status* and check whether there is a component having the status WARNING or ERROR.
3	Instrument Status Message Detector Detector not ready 	If so, double-click on the component icon in question to look up whether an instrument status message ① is displayed in OPUS. ☞ For information about the meaning of the instrument status messages refer to section 7.5.3.
4	INVENIO-S SN_28 DTC Diagnostics Messages Timestamp | Code | Level | Sender/Answer | Command | Message 20:50:08 | 20230 | S | Detector LN-MCT Narrow + Demodulated [PMA module] | Periodic initialization | Detector not ready RT-DLaTGS [Internal Pos.1] Detector selected | NO | DTC=0x4020 | PIC Vers 4.5 | SNo. DTR1299 | ECL05 | BoardType 027 Analog board settings | MUX=IR | TRW=OFF | HPF=OFF | GNS=1 | SG2=1 Error Level: No Error Messages | Channel right = Preamp A | Max Data Rate=80000 Hz Preamp board status | READY | PreampPower=OFF | PGN=0 (0..0) Detector properties | Range: 180..10000 | Vels: 400..10000..20000 | NL coef: 0wn, 1.000 | Recov. time: 3s Gains: 1.0/1.0/1.0/1.0 | Delays: 7500/7500/7500/7500ns	For more information about the component in question, open the corresponding diagnostic page of the spectrometer firmware and try to find a hint for the cause of the spectrometer problem. ☞ See section 7.2.4.

☞ For information about how to eliminate a certain fault, see section 7.5. If the solutions listed in this section do not eliminate a fault contact the Bruker service. For the Bruker service contact data, see section 1.6.

7.4 Remote fault diagnosis

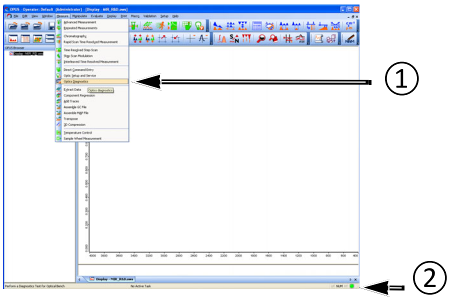
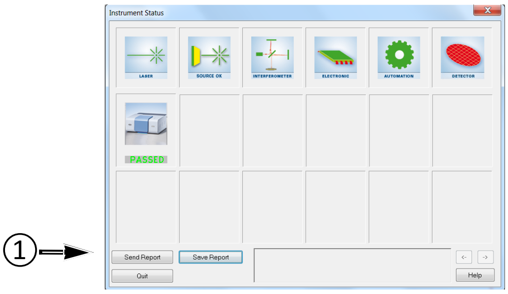
Remote fault diagnosis means that you send a complete spectrometer status report - a so called *Full Report* - by e-mail to Bruker. This report enables a Bruker service technician to perform a first remote fault diagnostics.

Depending on whether your spectrometer is connected to a network or network computer or a stand-alone computer, the procedure for sending the report is different. (For detailed information about the possible connection variants, see section 3.8.2.)

If your spectrometer is connected to a network computer or directly to a network...

☞ With OPUS, it is possible to send the full report by e-mail to Bruker with just the click of a button. **Important:** The usage of this function requires an e-mail program installed on the network computer and a set-up mail account.

Proceed as follows:

1		Open the OPUS software program, if not already done. Either select in the OPUS *Measure* menu the *Optics Diagnostics* function ① or click on the OPUS status light ②. ➣ Thereupon, the *Instrument Status* dialog opens.
2		Click on the *Send Report* button ①. ➣ As a result of this, the report is sent automatically by e-mail to *opusreports@bruker.com*.

If your spectrometer is connected to a stand-alone computer, proceed as follows:

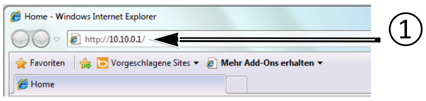
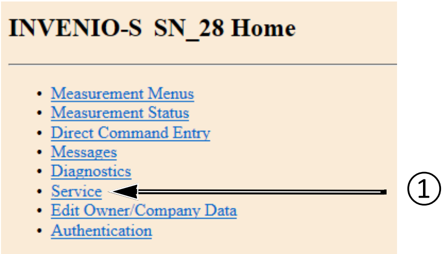
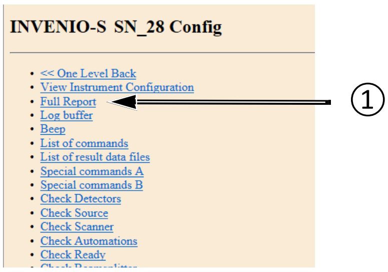
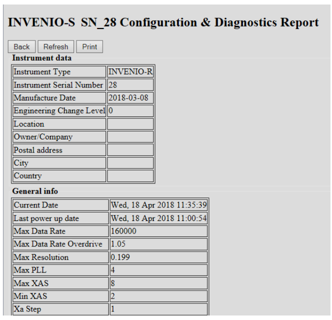
1. Generate a full report manually and save it. (See description below.)
2. Transfer the full report file to a network computer.

☞ Note: The network computer requires an e-mail program and a set-up mail account.

3. Send the full report by e-mail as an attached file to *opusreports@bruker.com*.

Generating and saving a Full Report

☞ It is highly recommended to generate and save the full report instantly after a spectrometer problem or failure has occurred. Otherwise, important information may be overwritten by newer ones.

1		Open an Internet browser. Enter the spectrometer IP address in the Internet browser entry field ① and press the ENTER key. • If the spectrometer is connected directly to an external PC, the standard IP address is 10.10.0.1. • In case of a DHCP-assigned IP address, you can enter instead of the IP address *invenio-s-SN* with *SN* being the serial number of the spectrometer in question. Note: You find the serial number of the spectrometer on the type label at the spectrometer rear side. • In case the spectrometer is directly connected to a network and a static IP address has been assigned using the FCONF program, you can retrieve the IP address as described in section E.6.
2		➢ Thereupon, the spectrometer home page opens. Click on *Service* ①.
3		Click on *Full Report* ①.
4	INVENIO-S SN_28 Configuration & Diagnostics Report **Instrument data** Instrument Type: INVENIO-R Instrument Serial Number: 28 Manufacture Date: 2018-03-08 Engineering Change Level: 0 Location: Owner/Company: Postal address: City: Country: **General info** Current Date: Wed, 18 Apr 2018 11:35:39 Last power up date: Wed, 18 Apr 2018 11:00:54 Max Data Rate: 160000 Max Data Rate Overdrive: 1.05 Max Resolution: 0.199 Max PLL: 4 Max XAS: 8 Min XAS: 2 Xa Step: 1	Save the full report as *.htm file for sending it as an e-mail attachment. Send the full report by e-mail as an attached file to *opusreports@bruker.com.*

7.5 Problem - possible cause - solution

7.5.1 Spectrometer problem indicated by a red status indicator LED

A red instrument status LED indicates an error. For example, this is the case when:

- an optical component (e.g. source, laser) fails or
- it does not achieve its performance specification

Note: In case of a red instrument status LED, measuring is **not** possible until the cause of the error is eliminated.

Defective or damaged component

In case of a defective or damaged component, it is highly recommended to open the OPUS dialog window *Instrument Status* to narrow down the problem. For diagnosing the fault, see section 7.2.2.

Possible causes	Solutions
If the **laser** is the cause of the problem the laser is defective. ➢ **Note:** This problem is indicated by the instrument status message *Laser is off or no laser signals*.	Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
If the **source** is the cause of the problem either: • the selected source is not installed or • the selected source is not properly installed or • the selected source is defective ➢ **Note**: This problem is indicated by the instrument status message *Source is broken or not connected*.	**Missing source:** Install the source. **Improperly installed source:** Check whether the source is installed properly and correct it, if required. **Defective source:** Order a replacement source. For the order number refer to section B.1. After receiving the replacement source, replace the defective source. ☞ For information about the proper installation and the replacement procedure, see the document *INVENIO - Source Replacement Instructions* which is added to the replacement source. ℹ Replacing the source is a recommended Bruker service delivery. ☞ For the Bruker service contact data, see section 1.6.

Possible causes	Solutions
If the **detector** is the cause of the problem:	
• the detector is defective: This problem is indicated by the instrument status message *Device not connected. No analog board selected*.	**Defective detector:** Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
• the MCT detector is not cooled down to its operating temperature. This problem is indicated by the instrument status message *Detector not ready*.	**MCT detector temperature is too high:** Fill liquid nitrogen into the MCT detector dewar. ☞ See section 5.11.
• the optional DigiTect-type detector is not properly installed: This problem is indicated by the instrument status message *Device not connected. No analog board selected*.	**Improperly installed DigiTect-type detector:** Check whether the detector is installed correctly and correct it, if required. See section 5.9.
If the **interferometer** (scanner) is the cause of the problem there are a number of possible causes.	Try to narrow down the trouble source by consulting the *Scanner Diagnostics Page*. (See fig. 7.6.) For error messages regarding the interferometer, see section 7.5.3.3. If you can not solve the problem, contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
If the **automation** is the cause of the problem there are a number of possible causes.	Try to narrow down the trouble source by consulting the *Automation Units Diagnostics Page*. (See fig. 7.9.) If you can not solve the problem, contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.

Possible causes	Solutions
If the **electronics** is the cause of the problem there are a number of possible causes. For example: • the electronics unit is defective or • there is a short circuit.	**Defective power supply unit:** Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6. **Short circuit:** Interrupt the mains power supply of the spectrometer immediately! If there are external accessories and/or components connected to the CAN bus port or any other spectrometer port, disconnect them. Then reconnect the spectrometer to the mains supply. If this action solves the problem the external circuitry has caused the short circuit. Otherwise, it is an internal problem of the spectrometer electronics. Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.

7.5.2 Spectrometer problem indicated by a yellow status indicator LED

A yellow instrument status indicates a warning. In case of a warning, measuring is still possible, but the reliability of the measurement is not ensured. For this reason, it is highly recommended to diagnose the cause of the warning and to eliminate it.

Possible causes	**Solutions**
Water vapor concentration inside the spectrometer is too high. Note: In this case, the instrument status message *Humidity out of range* is displayed in OPUS.	In general, the following actions can solve the problem: • Purging the spectrometer with dry air or nitrogen gas. (If the spectrometer is already purged check the degree of dryness of the purge gas.) See section 3.7.2. ➢ For information about how to connect the spectrometer to a purge gas supply line, see section 3.7. • Replacing the saturated cartridge(s) by new or regenerated cartridge(s). See section 6.2. ➢ Generally, the cartridges should be replaced about every 6 months. Either regenerate the desiccant and reuse it or order replacement cartridges and replace the cartridge(s). For the order number refer to section B.1. ➢ Purging the spectrometer with dry air reduces the water vapor concentration within a shorter period of time than the desiccant cartridges can do.
The validity period of an OVP test (OQ and/or PQ) of the currently selected measurement channel is expired. In this case, the measurement channel is question is labeled EXPIRED. ☞ See section 7.2.2.	Perform the PQ or OQ test for the currently selected measurement channel. ☞ For detailed information about OVP refer to the OPUS Reference Manual.

Possible causes	Solutions
The end of the specified lifetime of the source and/or laser is nearly reached.	First find out of which component - source or laser - the specified lifetime is nearly reached. For the component in question, the following instrument status message is displayed: *End of the average lifetime is nearly reached, spare part will be required*. ☞ See section 7.2.2 and section 7.2.3. **Source:** Order a replacement source. For the order number refer to section B.1. After receiving the replacement part, replace it. ☞ For information about the proper installation and the replacement procedure, see the document *INVENIO - Source Replacement Instructions* which is added to the replacement part. ℹ Replacing the source is a recommended Bruker service delivery. **Laser:** Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6. ➢ **Note:** Despite this warning message, measuring is still possible. To turn the OPUS status light green again click on the *Ignore* button in the *Instrument Status Message* dialog (fig. 7.3). The message will be repeated in certain intervals until the source or the laser has been replaced.

A failed validation test (PQ and/or OQ test)

☞ If a failed validation test is the cause of a yellow status indicator LED, see section 7.5.5 for troubleshooting.

7.5.3 Spectrometer problem indicated by an instrument status message in OPUS

7.5.3.1 Instrument status message regarding the laser

Instrument status message	**Possible causes**	**Solutions**
Laser is off or no laser signal.	Laser is not installed correctly. **OR** Power supply to the laser is interrupted. **OR** Laser is defective.	Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
End of average lifetime is nearly reached, spare part will be required.	The end of the specified lifetime of the laser is nearly reached. Note: If this message is displayed, first find out of which component - laser or source - the specified lifetime is nearly reached.	The laser needs to be replaced in the near future. Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6. ➢ **Note:** Despite this warning message, measuring is still possible. To turn the OPUS status light green again click on the *Ignore* button in the *Instrument Status Message* dialog (fig. 7.3). The message will be repeated in certain intervals until the laser module has been replaced.

7.5.3.2 Instrument status message regarding the source

Instrument status message	**Possible causes**	**Solutions**
Source is broken or not connected.	Source is not installed at all or not installed properly. **OR** Source is defective (e.g. burnt out).	Install the source properly. Order a spare source. For the order number refer to section B.1. After receiving the replacement source, replace it. ☞ For information about the proper installation and the replacement procedure, see the added document *INVENIO - Source Replacement Instructions*. ℹ Replacing the source is a recommended Bruker service delivery. ☞ For the Bruker service contact data, see section 1.6.

Instrument status message	**Possible causes**	**Solutions**
End of average lifetime is nearly reached, spare part will be required.	The end of the specified lifetime of the source is nearly reached. Note: If this message is displayed, first find out of which component - laser or source - the specified lifetime is nearly reached.	The source needs to be replaced in the near future. Order a spare source. For the order number refer to section B.1. After receiving the replacement source, replace it. ☞ For information about the proper installation and the replacement procedure, see the added document *INVENIO - Source Replacement Instructions*. ℹ Replacing the source is a recommended Bruker service delivery. ☞ For the Bruker service contact data, see section 1.6. ➢ **Note:** Despite this warning message, measuring is still possible. To turn the OPUS status light green again click on the *Ignore* button in the *Instrument Status Message* dialog (fig. 7.3). The message will be repeated in certain intervals until you have replaced the source.

7.5.3.3 Instrument status message regarding the scanner

Instrument status message	Possible causes	Solutions
Scanner initialization mode.	This error message appears only if you try to start a measurement while the spectrometer is still initializing. ➣ Also other error messages can be displayed. As in this case, there is not a spectrometer problem you can ignore them.	Before starting a measurement, wait until the spectrometer has completed the initialization successfully. ➣ As soon as the initialization is completed successfully, the spectrometer status indicator LED turns automatically to blue. Now you can start to measure.
Laser-A timing error / Laser-B timing error OR Laser-A modulation too small / Laser-B modulation too small OR Laser signals modulation too small OR Laser period too slow or modulation too small	Interferometer is out of adjustment caused by strong vibrations, for example.	Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.

Instrument status message	**Possible causes**	**Solutions**
Humidity out of range.	Water vapor concentration inside the spectrometer is too high.	In general, the following actions can solve the problem: • Purging the spectrometer with dry air or nitrogen gas. (If the spectrometer is already purged check the degree of dryness of the purge gas.) See section 3.7.2. ➢ For information about how to connect the spectrometer to a purge gas supply line, see section 3.7. • Replacing the saturated cartridge(s) by new or regenerated cartridge(s). See section 6.2. ➢ Generally, the cartridges should be replaced about every 6 months. Either regenerate the desiccant and reuse it or order replacement cartridges and replace the cartridge(s). For the order number refer to section B.1. ➢ Purging the spectrometer with dry air reduces the water vapor concentration within a shorter period of time than the desiccant cartridges can do.

7.5.3.4 Instrument status message regarding the detector

Instrument status message	**Possible causes**	**Solutions**
Detector not ready.	The MCT detector is not cooled down to its operating temperature.	Cool down the MCT detector by filling liquid nitrogen into the detector dewar. ☞ See section 5.11.
Device not connected. No analog board selected. OR No analog board found.	The optional DigiTect-type detector, which you have selected in OPUS, is not installed in the spectrometer.	Install the detector. ☞ See section 5.9.

7.5.4 No signal is detected or signal intensity is too low

Provided that the spectrometer and the PC are properly connected and switched on and the computer can access the spectrometer, this problem can have the following possible causes:

Possible Causes	**Solutions**
Beam path is blocked.	Check whether the IR beam is blocked in the sample compartment by an accessory or a sample or another object. Remove the sample / object and check the signal again.
In case of a MCT detector or a thermo-electrically cooled detector, the detector temperature is too high. ➢ This problem is indicated by the instrument status message *Detector not ready*.	**MCT detector:** Cool the MCT detector with liquid nitrogen. ☞ See section 5.11. **Thermo-electrically cooled detector:** Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
Detector is not or not properly installed / connected. ➢ This problem is indicated by the instrument status message *Device not connected. No analog board selected*.	**Internal detectors (optional DigiTect-type detector):** Install the detector properly. ☞ See section 5.9. **External detector:** Examine the cable connection at the detector as well as at the spectrometer rear side.
Detector oversaturation or A/D converter overflow	Reduce the source intensity either by using a smaller aperture, by attenuating the IR beam or by reducing the gain setting. ➢ These parameters (attenuator, aperture and gain) are set in the OPUS dialog *Measurement*, dialog page *Optics*. See section C.2.
Source is not or not properly installed or it is defective. ➢ These problems are indicated by the instrument status message *Source is broken or not connected.*	Install the source properly. If the source is defective, order a replacement source. For the order number refer to section B.1. After receiving the replacement source, replace it. ☞ For information about the replacement procedure and the proper installation, see the added document *INVENIO - Source Replacement Instructions*. ℹ Replacing the source is a recommended Bruker service delivery. ☞ For the Bruker service contact data, see section 1.6.

Possible Causes	Solutions
Beamsplitter is damage or the optical material of the beamsplitter has become opaque in the course of time and its opaqueness has reached such a degree that the transparency (infrared transmittance) is seriously reduced. Note: Especially hygroscopic materials (e.g. CsI, KBr) tend to become opaque.	Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
A temporary or permanent optics misalignment caused by strong shock.	Place the spectrometer on a vibration-free surface. In case of a temporary optics misalignment, this action can solve the problem. If this action does not solve the problem contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
The laser is the cause of the problem (e.g. the laser is defective). ➢ This cause is also indicated by a red spectrometer status LED and by the instrument status message: *Laser is off or no laser signals.*	Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.

7.5.5 A failed validation test

Validation test is a collective term for all tests (e.g. OQ test[1], PQ test[2]) that can be performed with OVP[3] for the purpose of the spectrometer validation[4].

☞ For detailed information about OVP refer to the OPUS Reference Manual.

Important note regarding the OQ test

☞ The resolution test, which is part of the OQ test protocol, requires a gas cell filled with CO at low pressure. If you do not have such a gas cell at your disposal, contact the Bruker service. For the contact data, see section 1.6.

Possible causes	Solutions
During the validation test measurements, an object (e.g. a sample) in the sample compartment has blocked the IR beam.	Take the sample / object out of the sample compartment and repeat the OVP test.
Source performance has decreased significantly because the end of its service lifetime is nearly reached. ➢ This problem is indicated by the following message *End of average lifetime is nearly reached, spare part will be required.* ➢ **Note:** To find out of which component - either laser or source - the end of the average lifetime is nearly reached, open in OPUS the *Instrument Status* dialog window. The component in question has the status WARNING.	Order a replacement source. For the order number refer to section B.1. After receiving the replacement source, replace the defective source. ☞ For information about the proper installation and the replacement procedure, see the document *INVENIO - Source Replacement Instructions* which is added to the replacement source. **i** Replacing the source is a recommended Bruker service delivery. ☞ For the Bruker service contact data, see section 1.6.
Sample compartment windows are dirty or their IR light transparency has declined significantly in the course of time. Note: Especially hygroscopic materials tend to become IR-non-transparent if exposed to humidity.	Order replacement windows. For the order number, see section B.2. After receiving them, replace them as described in section 6.4.

---

1. OQ - Operational Qualification (Normally, this test should be performed once a year or at least after the replacement of an optical spectrometer component.)
2. PQ - Performance Qualification (Normally, this test should be performed each day before you start your analytical work and after the replacement of an optical spectrometer component.)
3. OVP - OPUS Validation Program
4. Validating the spectrometer means to check whether the spectrometer system achieves the specified performance parameter values. The spectrometer validation ensures that the measurement results delivered by a validated spectrometer system are correct.

Possible causes	Solutions
The optical material of the beamsplitter is dirty or has become IR-non-transparent or the beamsplitter is damaged. Note: Especially hygroscopic materials tend to become IR-non-transparent if exposed to humidity.	Contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.
After you have filled liquid nitrogen in the MCT detector, you start the OVP test without waiting until the detector has reached its operating temperature.	After having filled in liquid nitrogen, wait about 20 minutes. Then, repeat the OVP test.
Ice formation on the MCT detector dewar. ➢ This problem becomes apparent by a failed ice band test. This test is part of the PQ test procedure.	Evacuate the MCT detector dewar as described in section 6.3. Afterwards, repeat the OVP test.
Air humidity content inside the spectrometer is too high. ➢ **Note:** This problem becomes apparent by a failed water vapor test. This test is part of the OQ test procedure.	Reduce the air humidity content inside the spectrometer by purging the spectrometer with dry air or nitrogen gas. Afterwards, repeat the OVP test. ☞ For information about purging the spectrometer, see section 5.8.
Interferogram peak position has shifted.	Save the new peak position using the OPUS software as described in section 5.10.3. Afterwards, repeat the OVP test.
If a failed OVP test has a different cause (e.g. detector sensitivity has weakened or interferometer is out of adjustment due to shock etc.) ...	... contact the Bruker service. ☞ For the Bruker service contact data, see section 1.6.

7.5.6 No communication between spectrometer and computer

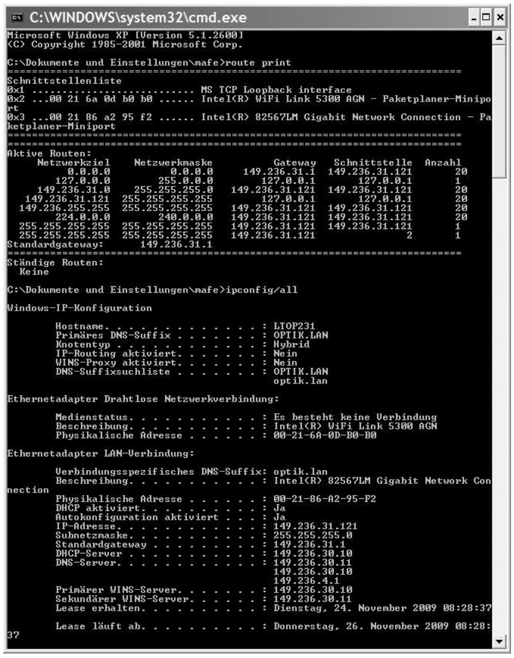
In case of communication problems between the spectrometer and an external PC, the troubleshooting procedure depends on the actually realized connection variant.

☞ For detailed information about this topic, see section 3.8.

Possible causes	**Solutions**
With regard to the existing connection variant, the wrong data cable type is used.	The data cable type (cross-over or straight), which has to be used, depends on the realized connection variant. ☞ For information about which data cable type has to be used for which connection variant, see section 3.8.1. Procure a data cable of the correct type. and replace the data cable.
Data cable connector is loose.	Check both data cable connectors for tight fit, i.e. at the Ethernet port at the spectrometer rear side and at the PC. Connect the data cable properly. ☞ See section 3.8.1.
Data cable is damaged.	Check the data cable for damages. If it shows signs of damages, replace it.
Spectrometer does not start up.	Check whether the spectrometer is connected to a mains socket outlet. ☞ See section 3.6. Check whether the mains supply meets the requirements. ☞ See section 3.5. Check whether the spectrometer is switched on. If not, do so now. ☞ See section 5.2. If these actions do not solve the problem contact the Bruker service. ☞ For the contact data, see section 1.6.
With regard to the realized connection variant, the wrong IP address has been assigned to the spectrometer. **Note:** The correct spectrometer IP address depends on the existing connection variant. (See section 3.8.5.)	Assign the correct IP address to the spectrometer. ☞ See section 3.8.6.
TCP/IP settings mismatch between spectrometer and computer/network.	☞ Refer to the documentation of the operating system Windows.

☞ Hint: If you do not succeed in solving the communication problem between spectrometer and PC, consult your network administrator. To provide the network administrator with the relevant information, proceed as follows:

1. Click in the Window desktop on the *Start* button.
2. Select *Run*.
3. Enter *cmd* and click OK.
4. Enter *route print* and press the ENTER key.
5. Then, enter i*pconfig/all* and press the ENTER key again.
6. Take a screenshot of the dialog (fig. 7.10) and provide it for your network administrator.



```
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.

C:\Dokumente und Einstellungen\mafe>route print
===========================================================================
Schnittstellenliste
0x1 ........................... MS TCP Loopback interface
0x2 ...00 21 6a 0d b0 b0 ...... Intel(R) WiFi Link 5300 AGN - Paketplaner-Minipo
rt
0x3 ...00 21 86 a2 95 f2 ...... Intel(R) 82567LM Gigabit Network Connection - Pa
ketplaner-Miniport
===========================================================================
===========================================================================
Aktive Routen:
     Netzwerkziel    Netzwerkmaske          Gateway   Schnittstelle  Anzahl
          0.0.0.0          0.0.0.0     149.236.31.1  149.236.31.121       20
        127.0.0.0        255.0.0.0        127.0.0.1       127.0.0.1       1
     149.236.31.0    255.255.255.0   149.236.31.121  149.236.31.121       20
   149.236.31.121  255.255.255.255        127.0.0.1       127.0.0.1       20
  149.236.255.255  255.255.255.255   149.236.31.121  149.236.31.121       20
        224.0.0.0        240.0.0.0   149.236.31.121  149.236.31.121       20
  255.255.255.255  255.255.255.255   149.236.31.121  149.236.31.121       1
  255.255.255.255  255.255.255.255   149.236.31.121               2       1
Standardgateway:      149.236.31.1
===========================================================================
Ständige Routen:
  Keine

C:\Dokumente und Einstellungen\mafe>ipconfig/all

Windows-IP-Konfiguration

        Hostname. . . . . . . . . . . . . : LTOP231
        Primäres DNS-Suffix . . . . . . . : OPTIK.LAN
        Knotentyp . . . . . . . . . . . . : Hybrid
        IP-Routing aktiviert. . . . . . . : Nein
        WINS-Proxy aktiviert. . . . . . . : Nein
        DNS-Suffixsuchliste . . . . . . . : OPTIK.LAN
                                            optik.lan

Ethernetadapter Drahtlose Netzwerkverbindung:

        Medienstatus. . . . . . . . . . . : Es besteht keine Verbindung
        Beschreibung. . . . . . . . . . . : Intel(R) WiFi Link 5300 AGN
        Physikalische Adresse . . . . . . : 00-21-6A-0D-B0-B0

Ethernetadapter LAN-Verbindung:

        Verbindungsspezifisches DNS-Suffix: optik.lan
        Beschreibung. . . . . . . . . . . : Intel(R) 82567LM Gigabit Network Con
nection
        Physikalische Adresse . . . . . . : 00-21-86-A2-95-F2
        DHCP aktiviert. . . . . . . . . . : Ja
        Autokonfiguration aktiviert . . . : Ja
        IP-Adresse. . . . . . . . . . . . : 149.236.31.121
        Subnetzmaske. . . . . . . . . . . : 255.255.255.0
        Standardgateway . . . . . . . . . : 149.236.31.1
        DHCP-Server . . . . . . . . . . . : 149.236.30.10
        DNS-Server. . . . . . . . . . . . : 149.236.30.11
                                            149.236.30.10
                                            149.236.4.1
        Primärer WINS-Server. . . . . . . : 149.236.30.10
        Sekundärer WINS-Server. . . . . . : 149.236.30.11
        Lease erhalten. . . . . . . . . . : Dienstag, 24. November 2009 08:28:37

        Lease läuft ab. . . . . . . . . . : Donnerstag, 26. November 2009 08:28:
37
```

Figure 7.10: Useful information for solving the communication problem between PC and spectrometer

A Specification

A.1 Spectrometer

Parameter	Specification
Weight	Basic spectrometer configuration: approx. 65 kg (Note: The exact weight depends on the individual instrument configuration.)
Dimensions	footprint: 68 cm (w) x 76 cm (d) height without touch panel PC: 32 cm height with touch panel PC: 50 cm height with open, large-sized sample compartment: 62 cm
Spectral range	**standard:** With the standard optical components (standard KBr beamsplitter, DLaTGS detector and MIR source) the following spectral range is achieved: MIR: 8,000 to 340 cm^{-1} **optional:** The available optional variants achieve the following spectral ranges: with broadband KBr beamsplitter: 11,000 to 350 cm^{-1} with CsI optics: 5,000 to 200 cm^{-1} with ZnSe optics (high humidity variant): 6,000 to 500 cm^{-1}
Spectral resolution	better than 0.4 cm^{-1}
Wavenumber accuracy	better than 0.01 cm^{-1} @ 1,554 cm^{-1}
Photometric accuracy	better than 0.1% T
Scan speed	6 velocities from 1.6 to 60 kHz (1.4 to 51 mm/sec opd)
Source	**standard:** MIR source, air-cooled **optional:** NIR source, air-cooled (for the spectrometer variant with broadband KBr beamsplitter only) ☞See also section 4.5.2.
Beamsplitter material	**standard:** KBr **optional:** KBr broadband, CsI, ZnSe ☞See also section 4.5.4.

Parameter	Specification
Detector	**standard:** DLaTGS detector with KBr window in case of the spectrometer variant with CsI optics: DLaTGS detector with CsI window **optional:** various MCT detectors ☞See also section 4.5.3.
Sample compartment window material	**standard:** KBr **optional:** CsI, ZnSe ☞See also section 4.5.5.
Laser	INVENIO S is a laser class 1 product according to EN 60825-1:2007. INVENIO S is equipped with a semiconductor VCSEL diode laser. Wavelength: 850nm Power output: 2mW Divergence angle: < 1mrad The laser diode itself is a laser class 3B product.
Interferometer	ROCKSOLID permanently aligned, wear-free and high stability interferometer
Sample compartment (large-sized)	Dimensions: 25.5 cm (W) x 27.0 cm (D) x 22.5 cm (H) The purgeable sample compartment is separated from the optical bench by windows or automatic shutters (The shutters are optional).
Electronics	Microprocessor-controlled optics bench with digital speed control, system diagnostics, advanced system check, 96 kHz A/D converter with 24 bit dynamic range.
Communication interface	Industry standard Ethernet connection, TCPIP protocol

A.2 Power supply

Parameter	Specification
Voltage	Spectrometer: 100 - 240 V AC, 50 - 60 Hz
Power consumption (basic spectrometer configuration without data system)	typical: 70 W maximum: 120 W
Overvoltage category	II according to EN 61010-1 or IEC 60664-1
Pollution degree	2 according to EN 61010-1 or IEC 60664-1
Protection class	I according to IEC 61140

➢ For the power supply specifications of the data system, see the corresponding user manual.

A.3 Purge gas supply

Parameter	Specification
Purge gas properties	air or nitrogen gas dry (dew point below -40°C) and clean (oil-free and dust-free) Recommendation: Use of DIN purity class 1-1-1 (dryness - residual oil - particles)
Pressure	max. 0.5 bar (7.25 psi) overpressure
Flow rate (controllable)	Recommended flow rate: 200 l/h. Flow rate must not exceed 500 l/h.

A.4 Environmental conditions

Parameter	Specification
Ambient temperature range	for spectrometer operation: 18°C to 35°C
Ambient temperature variations in case of long-term measurements	max. 1°C per hour and max. 2°C per day
Humidity (non-condensing)	≤ 80% (relative humidity)
Installation site	in a closed room, max. 2000 m above sea level

B Replacement parts

B.1 Consumables & components with a limited service lifetime

Order number	Replacement part
S 119/B	Desiccant cartridge (regenerable desiccant), package containing 2 cartridges
Q 328/I7	MIR source, mounted, 12 V
Q 428/I7	NIR source, mounted, 12 V

B.2 Windows

➢ Note: The windows listed in the table below are designed for both the sample compartment openings and the IR beam inlet and outlet ports.

Order number	Replacement part
F162-I11	ZnSe window (wedge 6 mrad, 45 x 3 mm)
F162-I5	KBr window (wedge 6 mrad, 45 x 3 mm)
F162-I7	CsI window (45 x 3 mm, protected)

B.3 Cleaning utilities

Order number	Item
1008033	Cleaning tissues for gentle cleaning of the ATR crystal

C Measurement parameters

C.1 General information

Before starting a measurement, you have to define the measurement parameters using the OPUS software. To do this, select in the OPUS *Measure* menu the *Advanced Measurement* function and enter adequate measurement parameter values. The selected parameter settings and values are stored in a XPM-file.

☞ For detailed information about this topic, refer to the OPUS Reference Manual.

C.2 Default parameter values and settings

For INVENIO S, the following xpm-files are delivered with OPUS:

- MIR_TR.XPM (for MIR measurements in transmittance)
- MIR_ATR.XPM (for MIR measurements with an ATR accessory)
- MIR_ATR_preview.XPM (for MIR measurements with an ATR accessory and with the preview mode being activated))
- MIR_DRIFT.XPM (for MIR measurements in diffuse reflectance)
- MIR_Refl_30.XPM (for MIR measurements in reflectance; the accessory is designed for a reflection angle of 30°.)

These XPM-files include the standard parameter settings and values for dedicated types of measurement (e.g. transmittance, reflectance, ATR).

Take into consideration that depending on the actual spectrometer configuration, different measurement parameter settings and values may apply. Especially the optics parameter settings depend on the spectrometer configuration. In this case, you have to adapt the parameter settings and values correspondingly.

The following table lists the standard parameter values and settings which apply to the standard spectrometer configuration for a MIR measurement in transmittance.

Advanced parameters	**Settings and values**
Resolution	4
Sample/Background Scan Time	6 scans
Save Data	from 7500 to 400cm^{-1}
Result Spectrum	Transmittance
Data Blocks to be saved	Transmittance, Single Channel and background
Optics Parameter	**Settings**
Source Setting	MIR
Beam splitter	KBr
Optical Filter Setting[a]	open

Attenuator[b]	open
Aperture Setting[c]	6mm
Sample/Background Measurement Channel	Sample Compartment
Detector Setting	RT-DLaTGS (Internal Pos. 1)
Scanner Velocity	10 kHz
Sample Signal Gain	automatic
Background Signal Gain	automatic
Delay after Device Change	3
Delay before Measurement	0
Acquisition Parameters	**Setting**
Wanted High Frequency Limit	15.800cm^{-1}
Wanted Low Frequency Limit	0cm^{-1}
High Pass Filter	open
Low Pass Filter	10kHz
Acquisition Mode	Double Sided - Forward/Backward
Correlation Mode	OFF
FT-Parameters	**Settings**
Phase Resolution	16cm^{-1}
Phase Correction Mode	Power Spectrum
Apodization Function	Blackman-Harris3-Term
Zerofilling Factor	2

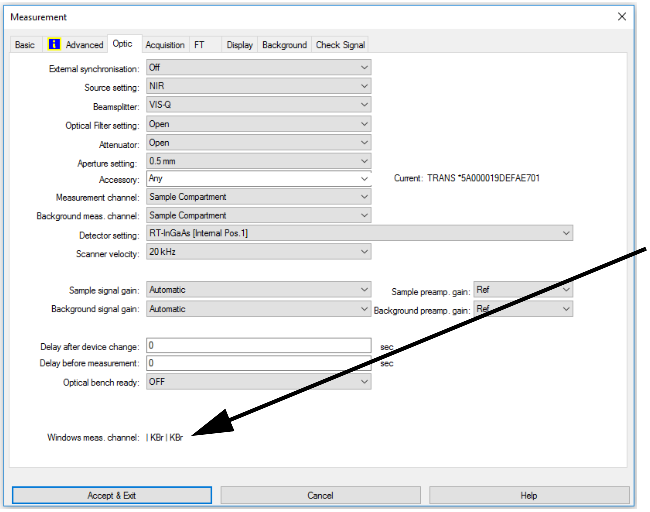
a. Note: The available optical filter options (NG4, NG9, NG11 and polystyrene) are used for OQ and PQ tests only. When such a test is running, the correct filter is moved automatically in the beam path, i.e. it does not need to be selected explicitly by the user. Normally, these optical filters are not intended for spectroscopic measurements. For this reason, select by default the optical filter setting Open when defining the measurement parameters. Note: There are vacant filter wheel positions which can be equipped with optional filters (filter diameter: 25 mm), if desired. They can be used for customer-specific applications.

b. The attenuator is a sieve wheel with different sieve sizes for an additional attenuation of the IR beam The IR beam can be attenuated down to 50%, 25%, 12.5% and 6.26%. The attenuator wheel is an optional feature. Attenuating the IR beam by means of the attenuation wheel is advisable in the following cases: 1) to avoid a detector oversaturation, 2) in case of a very intense source and 3) if you want to attenuate the IR beam without changing the aperture.

c. By default, the aperture wheel has 12 occupied positions which allow for the following aperture settings: 0.25, 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 5, 6, and 8 mm. The optimal aperture setting depends mainly on the detector and the source which are currently used and on whether the measurement is to be performed using a special accessory or not. As a rough guideline: The more sensitive a detector is the smaller the aperture should be (e.g. MCT: ca. 2 mm). In case of an accessory having a small measurement spot, select a small aperture (e.g. A518, reflection unit, grazing incidence 80°: < 1 mm). Note: In addition to the 12 default aperture wheel positions, there are four vacant aperture wheel positions which can be equipped with customer-specific apertures, if desired. These optional aperture settings are selectable by direct commands.

C.3 Optic parameter *Windows Measurement Channel*

In the *Measurement* dialog on the *Optics* page, the installed windows are displayed as follows:



External synchronisation: Off
Source setting: NIR
Beamsplitter: VIS-Q
Optical Filter setting: Open
Attenuator: Open
Aperture setting: 0.5 mm
Accessory: Any
Current: TRANS *5A000019DEFAE701
Measurement channel: Sample Compartment
Background meas. channel: Sample Compartment
Detector setting: RT-InGaAs [Internal Pos.1]
Scanner velocity: 20 kHz
Sample signal gain: Automatic
Sample preamp. gain: Ref
Background signal gain: Automatic
Background preamp. gain: Ref
Delay after device change: 0 sec
Delay before measurement: 0 sec
Optical bench ready: OFF
Windows meas. channel: | KBr | KBr

Display of the installed windows

Note: The order in which the windows are displayed in OPUS corresponds with the optical beam path starting from the IR source to the detector.

☞ For information about the optical beam path, see section 4.6.

Figure C.1: OPUS Measurement dialog - Optics page

D Dimensional drawings

D.1 INVENIO S without touch panel PC

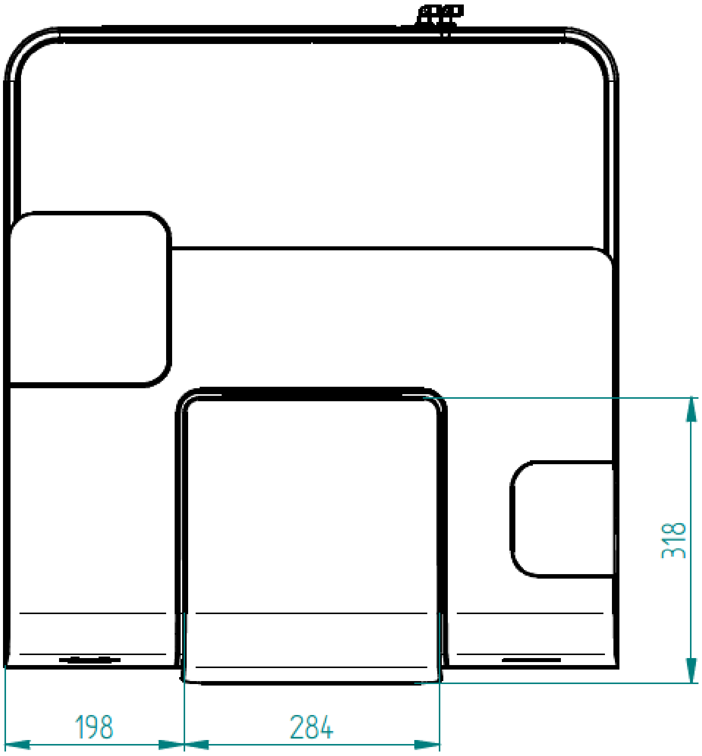


Figure D.1: INVENIO S without touch panel PC - Top view

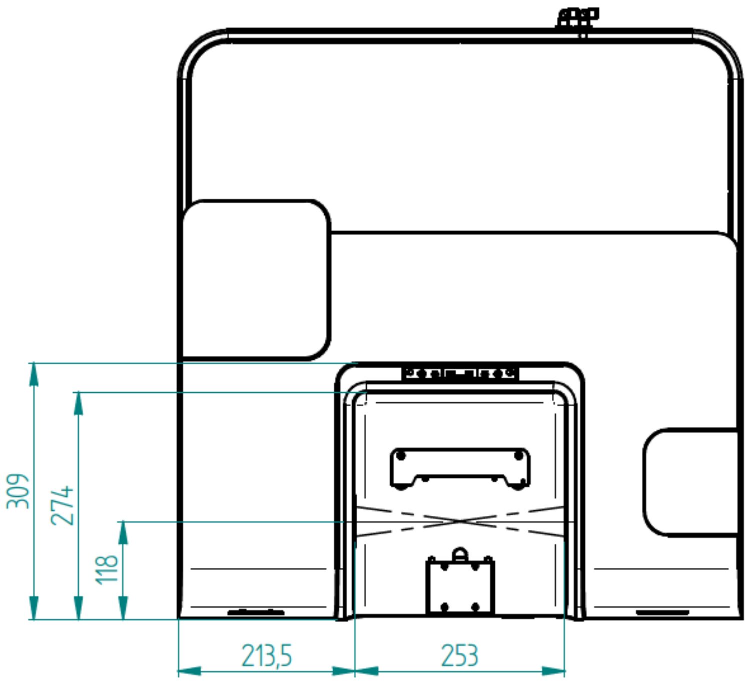


Figure D.2: Top view showing sample compartment dimensions

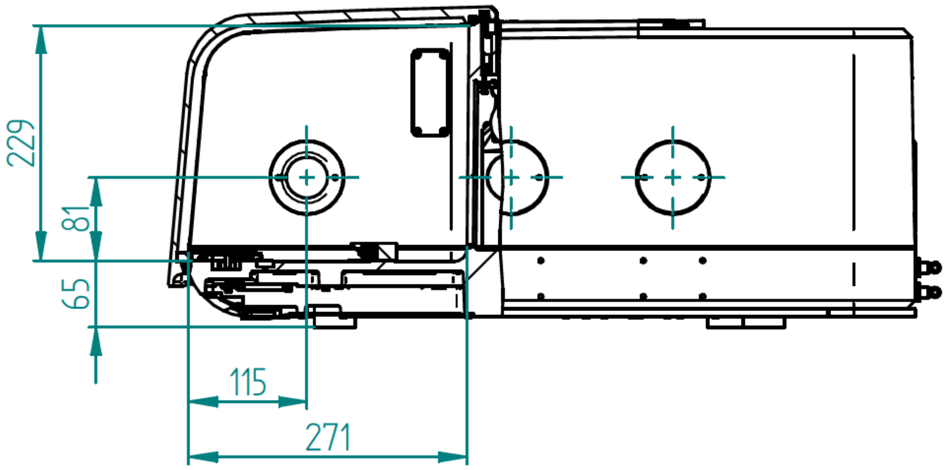


Figure D.3: INVENIO S without touch panel PC - Right side view showing the sample compartment dimensions

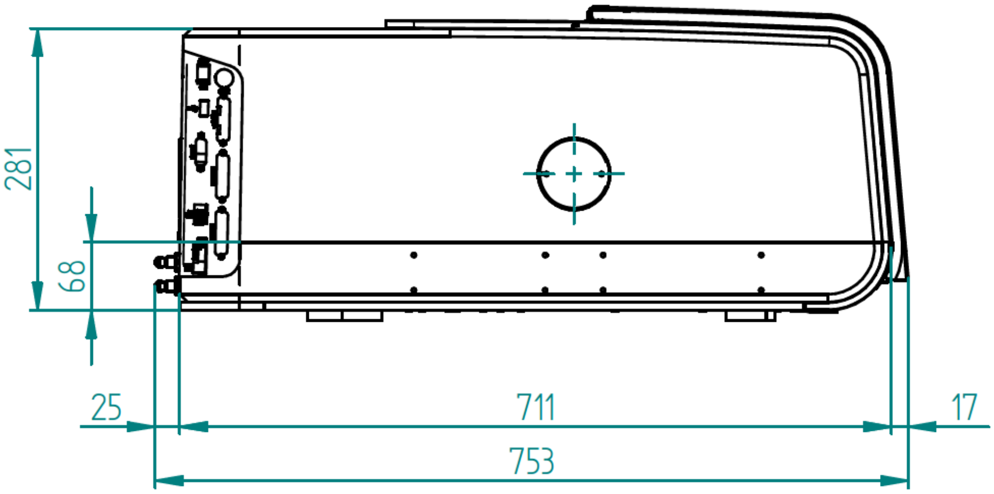


Figure D.4: INVENIO S without touch panel PC - Left side view

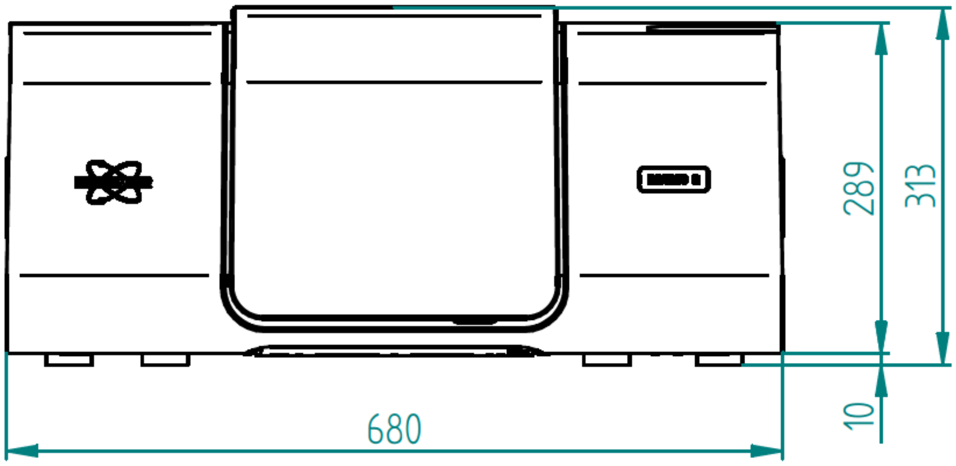


Figure D.5: INVENIO S without touch panel PC - Front view

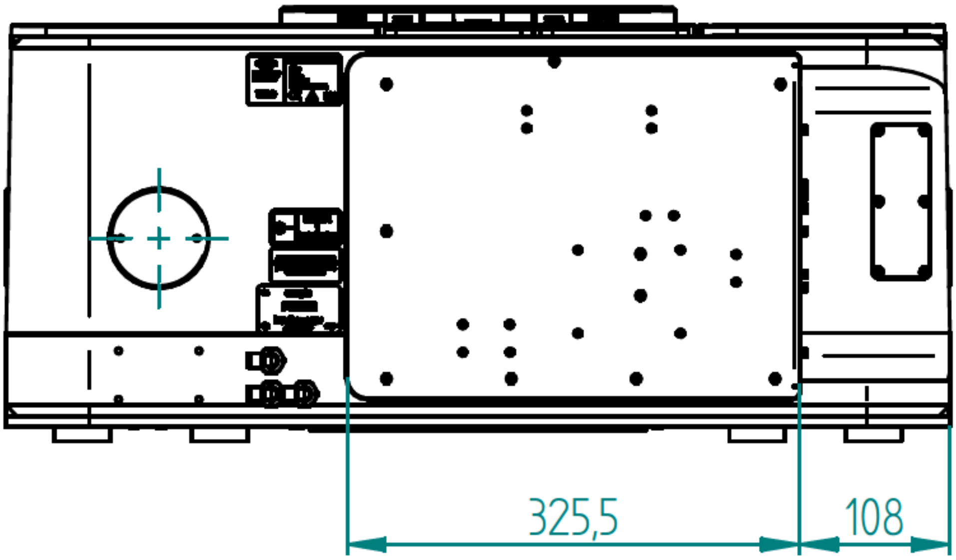


Figure D.6: INVENIO S without touch panel PC - Rear view

D.2 INVENIO S with touch panel PC

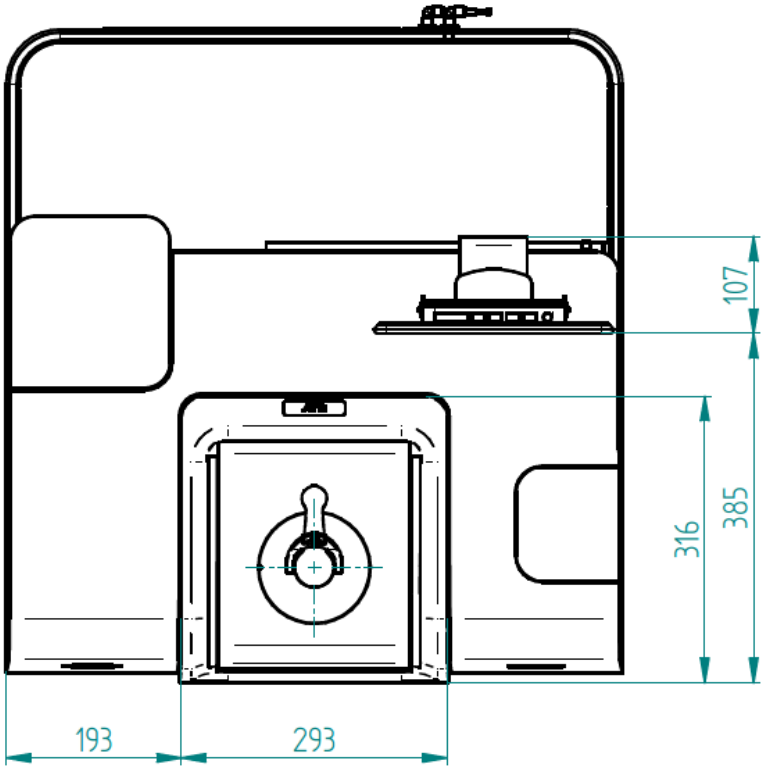


Figure D.7: INVENIO S with touch panel PC and ATR unit - Top view

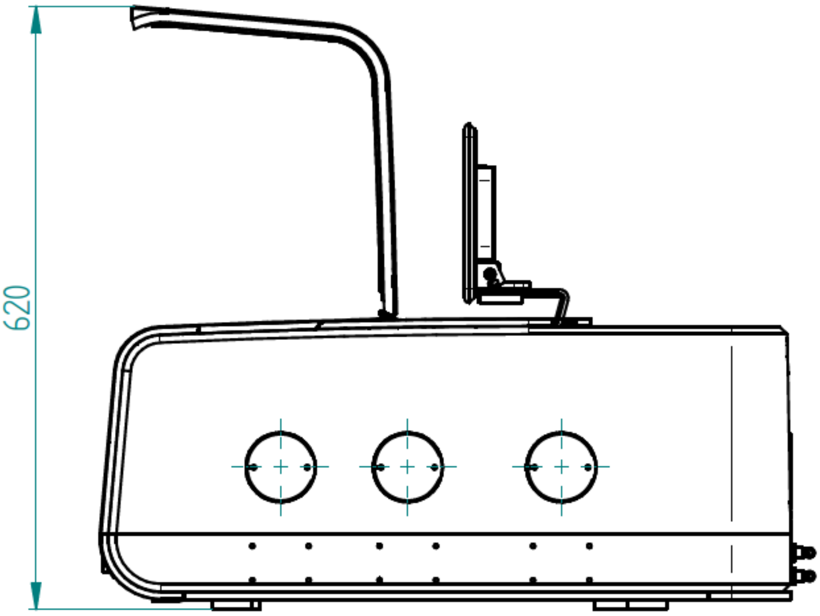


Figure D.8: Right side view with open sample compartment cover

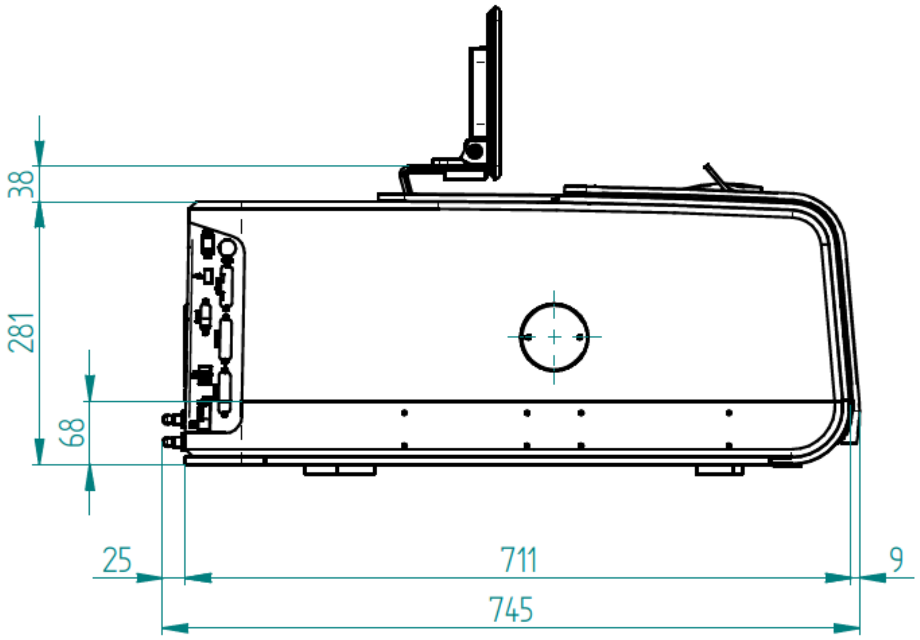


Figure D.9: INVENIO S with touch panel PC - Left side view

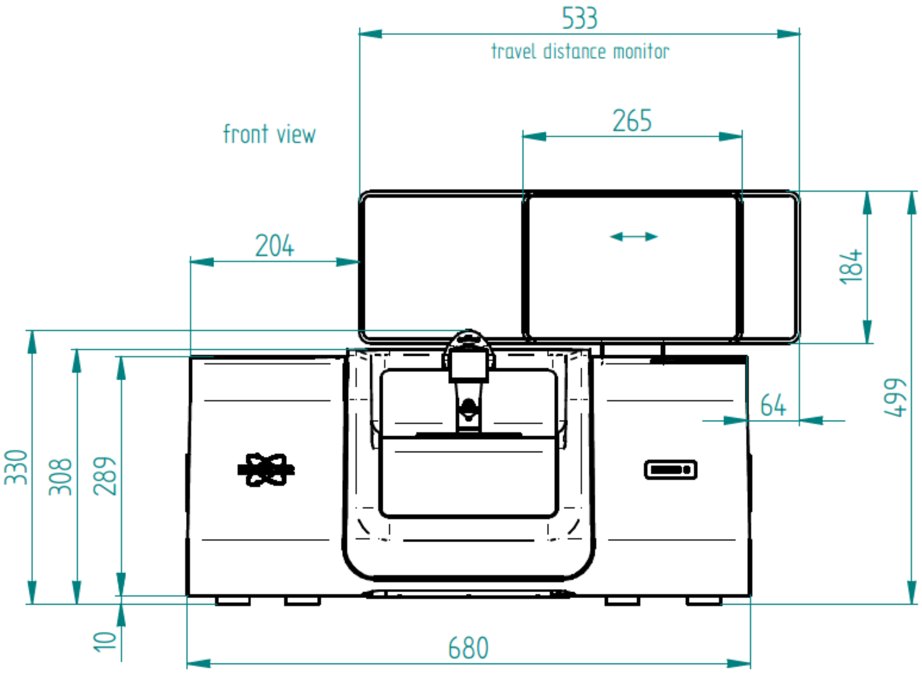


Figure D.10: INVENIO S with touch panel PC and ATR - Front view

E Spectrometer firmware

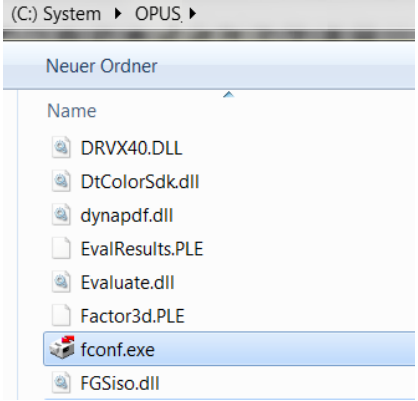
E.1 General information

All spectrometer-firmware-related tasks are executed by the FCONF program (Firmware Configuration Tool), namely:

- updating the firmware,
- restoring a previous firmware version,
- backing up the current firmware version,
- initializing the firmware (For service purposes only!),
- running a custom script (For service purposes only!).
- assigning a new IP address to the spectrometer (See section 3.8.6.)

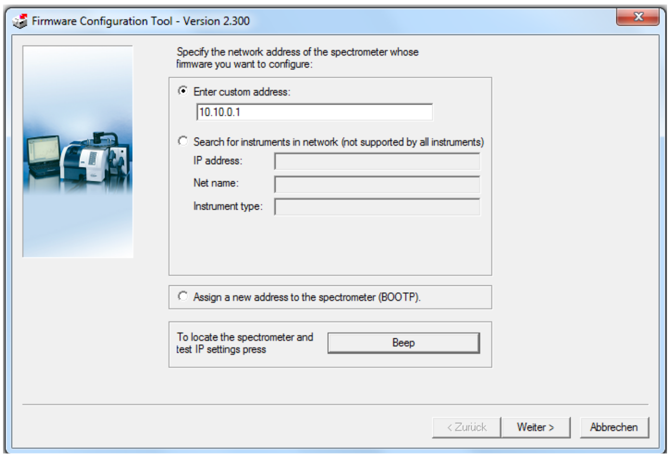
E.2 Starting the FCONF program

1. Browse in the file manager to *C:\Program\Bruker\ OPUS [current version]* and start the FCONF program by double-clicking on *fconf.exe.*



☞ Note: In case of updating the spectrometer firmware, the firmware update is typically delivered on CD or by e-mail. If the firmware update has been delivered on a CD, start the FCONF program directly from the CD by double-clicking on the *fconf.exe* file and proceed as described below. If the firmware update has been delivered via e-mail, first store the delivered files into a temporary directory. Then, proceed as described below.

➢ Thereupon, the following dialog opens:



Firmware Configuration Tool - Version 2.300

Specify the network address of the spectrometer whose firmware you want to configure:

● Enter custom address:
10.10.0.1

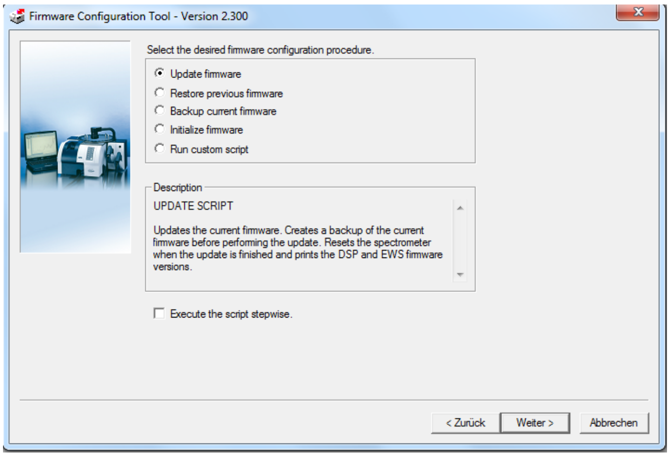
○ Search for instruments in network (not supported by all instruments)
IP address:
Net name:
Instrument type:

○ Assign a new address to the spectrometer (BOOTP).

To locate the spectrometer and test IP settings press

2. Specify the spectrometer of which the firmware is to be updated. To do this, activate the *Enter custom address* option button and enter the corresponding IP address in dotted notation. (Note: The spectrometer IP address depends on the realized connection variant. For more information, see section 3.8.5.)
3. After having entered the IP address, check whether the intended spectrometer is addressed by clicking on the *Beep* button. The addressed spectrometer will beep shortly three times.
4. Click the *Next* button.

E.3 Updating the spectrometer firmware



Firmware Configuration Tool - Version 2.300

Select the desired firmware configuration procedure.

● Update firmware
○ Restore previous firmware
○ Backup current firmware
○ Initialize firmware
○ Run custom script

Description

UPDATE SCRIPT

Updates the current firmware. Creates a backup of the current firmware before performing the update. Resets the spectrometer when the update is finished and prints the DSP and EWS firmware versions.

☐ Execute the script stepwise.

1. Activate the *Update firmware* option button.
2. Click on the *Next* button.
3. Select the directory (run folder) in which the backup data are to be stored.

☞ Note: It is recommended to accept the displayed default directory.

4. Follow the next on-screen instructions.

A spectrometer firmware update involves the following steps:

- At first, the FCONF program backs up the current version in case the update-version does not ensure a trouble-free operation so that the firmware needs to be restored again. (For information about how to restore a previous firmware version, see section E.2.)
- Then, the FCONF program updates the current spectrometer firmware version.
- Afterwards, it resets the spectrometer.

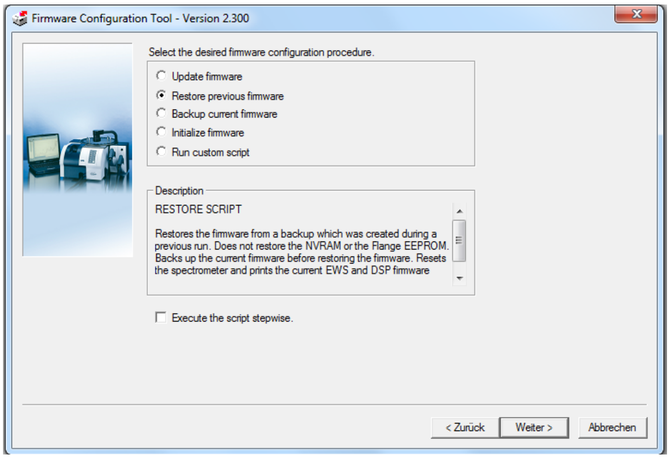
➢ The update procedure may take several minutes, depending on the available bandwidth and the amount of files to be updated.

➢ After the firmware update has been completed successfully, a corresponding message appears.

➢ In case of error during the update procedure, the FCONF program terminates the procedure and proposes to restore the previous firmware version. (For information about how to restore a previous firmware version, see section E.2.)

E.4 Restoring a previous firmware version

☞ You can restore only a firmware version which has been backed up before.



Select the desired firmware configuration procedure.

○ Update firmware
● Restore previous firmware
○ Backup current firmware
○ Initialize firmware
○ Run custom script

Description

RESTORE SCRIPT

Restores the firmware from a backup which was created during a previous run. Does not restore the NVRAM or the Flange EEPROM. Backs up the current firmware before restoring the firmware. Resets the spectrometer and prints the current EWS and DSP firmware

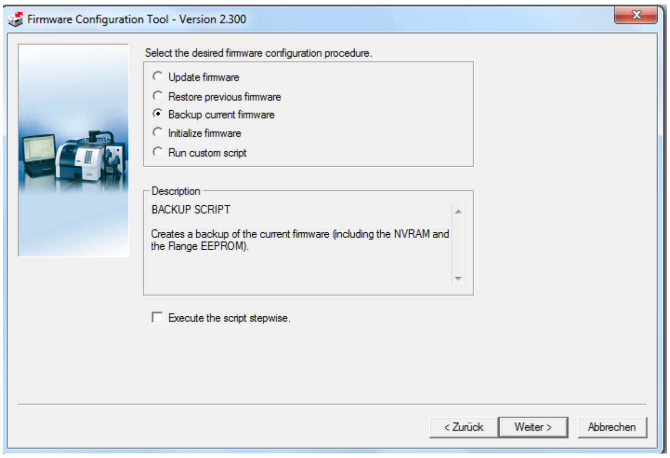
☐ Execute the script stepwise.

1. Activate the *Restore previous firmware* option button.
2. Click on the *Next* button.
3. Select the directory (run folder) which contains the firmware version you intend to restore.
4. Follow the next on-screen instructions.

Restoring a previous spectrometer firmware version involves the following steps:

- At first, the FCONF program backs up the current version.
- Then, the FCONF program restores the spectrometer firmware on the basis of a previous firmware version which the user has been backed up before.
- Afterwards, it resets the spectrometer.

E.5 Backing up the current spectrometer firmware version



Firmware Configuration Tool - Version 2.300

Select the desired firmware configuration procedure.

○ Update firmware
○ Restore previous firmware
● Backup current firmware
○ Initialize firmware
○ Run custom script

Description

BACKUP SCRIPT

Creates a backup of the current firmware (including the NVRAM and the Flange EEPROM).

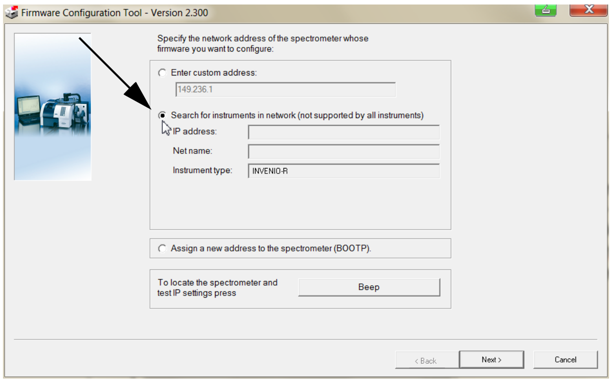
☐ Execute the script stepwise.

1. Activate the *Backup current firmware* option button.
2. Click on the *Next* button.
3. Follow the on-screen instructions.

E.6 Retrieving the spectrometer IP address

In case you need to know the currently assigned IP address of the spectrometer, you can retrieve it by proceeding as follows:

1. Activate the *Search for instrument in network* option button.



Firmware Configuration Tool - Version 2.300

Specify the network address of the spectrometer whose firmware you want to configure:

○ Enter custom address:
149.236.1

● Search for instruments in network (not supported by all instruments)
IP address:
Net name:
Instrument type: INVENIO-R

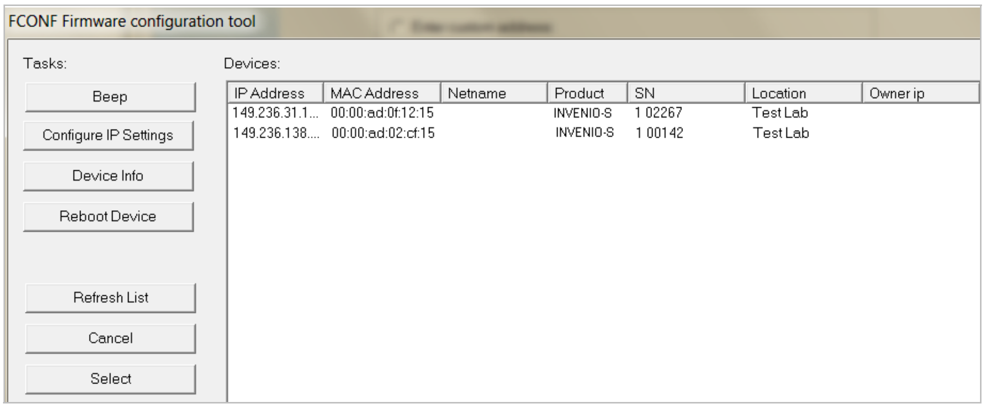
○ Assign a new address to the spectrometer (BOOTP).

To locate the spectrometer and test IP settings press

2. Click the *Next* button.

➢ *FCONF starts to search for all spectrometers connected to the network, or directly to a PC.*

The search result is displayed as follows:



IP Address	MAC Address	Netname	Product	SN	Location	Owner ip
149.236.31.1...	00:00:ad:0f:12:15		INVENIO-S	1 02267	Test Lab	
149.236.138....	00:00:ad:02:cf:15		INVENIO-S	1 00142	Test Lab	

3. To find out which of the displayed IP addresses belongs to which spectrometer, select an entry in the list box and click the *Beep* button. Thereupon, the spectrometer in question beeps once. In doing so, you can find out the IP address of a certain spectrometer.
4. Make a note of the IP address you are looking for.

F Sample preparation

F.1 General information

Proper sample preparation is crucial to obtain good and meaningful spectra. This section describes several sample preparation techniques that cover a wide range of samples. It will give you some help in choosing the most suitable sample preparation technique for a given sample.

The adequate sample preparation technique depends on the state of aggregation and the spectral absorptivity of the sample. Regardless of the state of aggregation, the sample material has to be homogeneous because variations in concentration or composition within the sample area to be analyzed can result in misleading or erroneous data. Sometimes the trial-and-error procedure is required to obtain an acceptable spectrum.

F.1.1 State of aggregation

Depending on the state of aggregation of the sample, there are different sample preparation and measurement techniques. If you have to analyze a solid sample in transmission you can either prepare a solution, a Nujol mull or a KBr pellet. Liquid samples can be analyzed either as a thin film between plates or in a liquid cell. Gaseous samples require dedicated cells with different path lengths.

F.1.2 Absorptivity

The absorptivity of the sample is a critical factor in choosing a suitable sample preparation method. To get a meaningful spectrum of a strongly absorbing sample, the sample has to be either:

- very thin or
- diluted by a solvent or powder that is not strongly absorbing.

According to Lambert Beer’s Law, the absorbance (i.e. peak intensity) in an absorbance spectrum is directly proportional to the component concentration in the sample, pathlength of the sample and the absorptivity.

$$A = \varepsilon b C$$

Symbol	Description	Typical measuring units
A	Absorbance at a given wavelength	None
ε	Molar absorptivity (a proportionality constant)	$l \cdot mol^{-1} \cdot cm^{-1}$
b	Pathlength of the sample (cell length for samples in a cell or sample thickness for films, pressed pellets)	cm
C	Component concentration in the sample	mol/l

If the absorbance *A* (i.e. peak intensity) is too strong, decrease the sample concentration *C* by diluting it or diminish the pathlength *b* by reducing the sample thickness. If the absorbance *A* (i.e. peak intensity) is too weak, increase the sample concentration *C* or the pathlength *b* correspondingly to obtain a reasonable peak intensity.

To find out whether a sample is strongly absorbing in the wavelength range of interest or not you have to acquire a test transmission spectrum. Figure F.1 shows a transmission spectrum of a strongly absorbing sample.

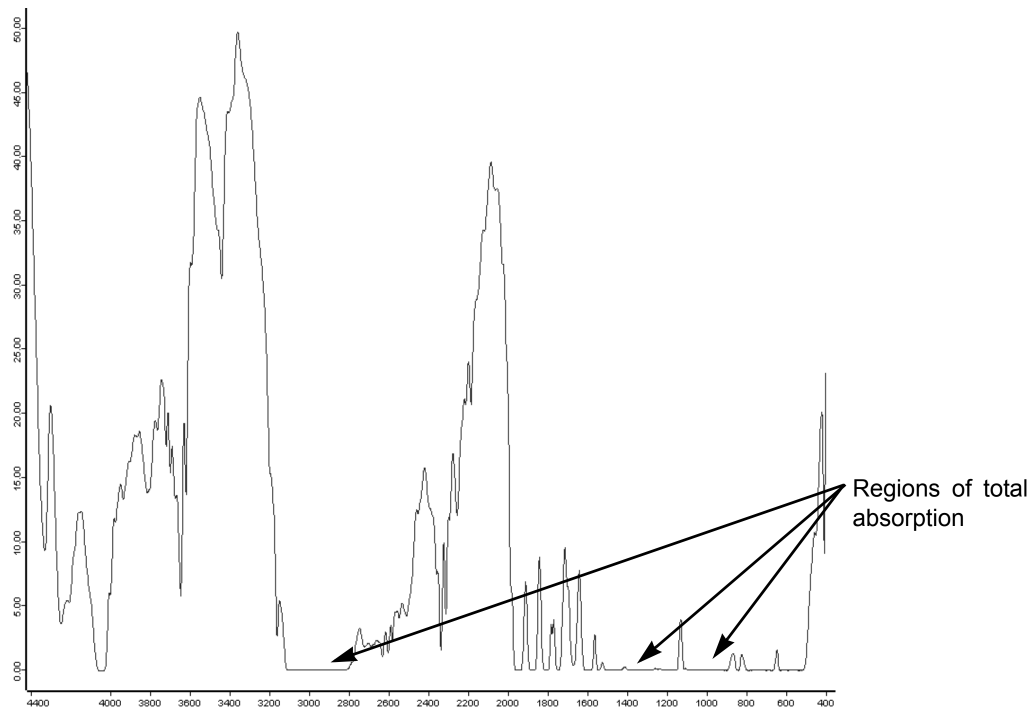


Figure F.1: Transmission spectrum of a strongly absorbing sample

F.2 Sample preparation techniques

There is a large number of possible sample preparation techniques. For lack of space, however, not all possible techniques can be described in detail in this chapter. Therefore, we restrict our explanations only to the most common techniques. (For more detailed information about this topic refer to the relevant specialist literature[1].) Moreover, we give you a general guideline for choosing the adequate sample preparation technique.

To find the most adequate method we recommend trying several sample preparation techniques and acquiring spectral data. On the basis of these data, you can assess which sample preparation technique is the most suitable one for your application. In case of doubt ask your application specialist.

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[1] e.g. Günzler, Helmut / Gremlich, Hans-Ulrich (2002): IR Spectroscopy - An Introduction. Weinheim: WILEY-VCH Verlag.

Some of the most common sample preparation techniques are:

- No sample preparation (e.g. self supporting film or measurement using a micro-ATR accessory)
- Thin film of liquid sample solution between two IR-transparent plates[1]
- Preparing a sample solution
- Preparing a Nujol mull[2]
- Pressing a KBr pellet
- Liquid cell and gas cell

➢ Most of the described sample preparation techniques involve the use of hygroscopic materials (such as NaCl or KBr), i.e. if these materials come in contact with water, they begin to dissolve or become opaque and thus, impair the measurement results. Therefore, avoid all sources of water and even alcohols (ethanol and methanol).

F.2.1 No sample preparation

The easiest samples to analyze are film and polymer samples with a thickness of less than approx. 100 micrometers. They can be simply placed in a magnetic holder and immediately scanned. The same procedure can be used for samples which can be sliced to an appropriate thickness.

A large number of solid and liquid samples can also be analyzed without requiring a preparation using a micro-ATR accessory. Attenuated Total Reflectance (ATR) units are a very versatile accessory for FTIR measurements. In many cases, the micro-ATR unit can be used for liquid and semi-liquid materials instead of the constant path transmission cells and the salt plates. In addition, this measurement accessory can also be used for analyzing polymer films, pastes and powders. Due to the reproducible effective path-length, they are well suited for both qualitative and quantitative analyses. Depending on the sample material and the objective of the analysis, there are different ATR-crystal materials (e.g. ZnS, ZnSe, Ge and diamond). The sample penetration depth ranges between 0.1 and 2µm and depends on the wavelength, the refractive index of the ATR-crystal material and the incidence angle of the beam. (For more information about attenuated total reflectance refer to the respective specialist literature.)

F.2.2 Thin film between plates

Preparing a thin film of a liquid sample between two IR-transparent plates is an easy sample preparation method. Choose this method if your sample is either a liquid or an oil. An advantage of this method is that only a small amount of the sample is required.

- Apply a drop of the sample on one of the plates using a pipet.
- Place a second plate on the top and make a quarter turn to obtain a nice even film of the liquid sample. Sandwich the plates carefully together to remove all air bubbles. Note that these plates are very fragile and can break easily. (The space between the two plates is very small (typically < 0.01mm).
- If the sample amount proved to be too much, separate the plates, wipe one side clean and fit the plates together again.
- Slot the plates in the sample holder of the spectrometer and start the measurement.

---

[1] i.e. IR-transparent within the frequency range of interest

[2] A mull is a mixture (more precisely a suspension) of two substances, one of which (i.e. the sample) is finely divided and dispersed in the other (e.g. the paraffin oil Nujol).

➢ The plates (made of NaCl or KBr) are extremely moisture sensitive. Therefore, do not use samples that contain water, keep the plates always dry, clean them only with chloroform or high purity acetone and polish them carefully after each use. In the course of time they will absorb moisture from the atmosphere and deteriorate. Therefore, proper storage (e.g. in an desiccator) is extremely important.

F.2.3 Solid sample as sample solution

Use this sample preparation method if your sample is a soluble solid (e.g. a soluble powder). To obtain an IR spectrum, you have to prepare a concentrated solution of your sample using a suitable solvent. The concentration of the solution needed for a good spectrum depends on the sample.

- Dissolve the sample or sample powder in a solvent and apply the sample solution between two support plates, as described above. Depending on the available amount of sample material you can either apply a small amount of your sample powder directly on the plate and add one drop of the solution or dissolve the sample in a test tube and apply the solution with a pipet on the plate.
- A second variant is to apply the sample solution on an IR-transparent plate and allow the solvent to evaporate leaving a thin sample film on the plate. Then, slot the plate in the sample holder of the spectrometer and start the measurement.
- A third variant is to fill the sample solution in a liquid cell and acquire a sample spectrum. To acquire a background spectrum measure the liquid cell containing only the solvent. The volumes of these liquid cells are between 0.1 and 1ml. Microcells with a much lower capacity are also available.
- Do not forget to acquire a background spectrum from the solvent as well.

➢ The plates (made of NaCl or KBr) are extremely moisture sensitive. (See above.)

The major problem in preparing a solution is choosing an appropriate solvent. Most solvents have a strong absorptivity and so their absorption bands will superimpose those of the solute. Therefore, you have to ensure that the used solvent is not strongly absorbing in the wavelength range of interest. Use only spectrophotometrically pure solvents and solvents that are not infrared active in the spectral region of interest.

No solvent is perfect but if some information about the sample is known, the solvent can be chosen accordingly. Commonly used solvents are carbon tetrachloride, carbon disulphide, chloroform, cyclohexane, acetonitrile, and tetrachloroethylene. Never use water as solvent because, firstly, it will dissolve the salt plates and secondly, it exhibits a broad OH-peak. Consult the relevant reference books for the absorptivity of the various solvents.

F.2.4 Preparing a mull

This sample preparation method is suitable if the solid sample can be ground into fine particles but a suitable solvent is not available. In this case the sample powder is suspended in a mulling agent (i.e. a liquid in that the solid is not soluble). A suitable mulling agent is Nujol, a paraffin oil, which is transparent in the infrared region, except for narrow bands at 2900, 1450 and 1375cm^{-1}. (An alternative mulling agent, which does not absorb in these regions, is a perfluorokerosene, such as Fluorolube.)

The advantage of this technique is that it is a relatively quick and simple procedure. The disadvantage is the interference resulting from the absorption bands of the mulling agent. (Both Nujol and Fluorolube have characteristic spectral features and in most cases have to be used as a pair in order to generate a complete MIR spectrum. Nujol is used below 1330cm-1, Fluorolube above 1330cm^{-1}.)

- Put a small amount of your solid sample in an agate mortar.
- Grind the sample thoroughly into fine powder (particles smaller than 500 mesh) using a pestle.

➢ A common mistake when preparing a Nujol mull is to spend too little time grinding the powder. Note that a mull prepared from a coarsely ground solid will yield only a poorly resolved spectrum. Grinding the sample into very fine particles is also important to reduce light scattering and salt plate scratching.

- Add 1 or 2 drops of Nujol. Be careful not to add too much Nujol.
- Mix the ground sample with the mulling agent until a uniform paste with a vaseline-like consistency is formed.
- Apply some mull on the surface of a NaCl plate using a suitable tool (e.g. a small spatula or a rubber policeman). Be careful not to scratch the plate.
- Place the second plate over the mull. To ensure an even and thin sample thickness between the plates, rotate and press the plates together in order to squeeze out the excess of the paste. Exclude also air bubbles.
- Slot the plates in the plate holder installed in the spectrometer sample compartment and start the measurement.
- Do not forget to acquire also a background spectrum of the pur Nujol.

F.2.5 Pressing a KBr pellet

This sample preparation technique is very suitable for solid samples in terms of the information yield from an IR spectrum because KBr is significantly more IR transparent than most solvents or Nujol oil. KBr has no absorption in the region 4000cm^{-1} to 250cm^{-1} so that a good sample spectrum (i.e. a spectrum that does not contain spectral information about the dispersing agent) is obtained.

The success of this technique strongly depends on the grain size of the ground sample. Grind the sample as fine as possible (particle size of at least 200 mesh, better 500 mesh) to minimize the infrared light scattering on the particle surface, also called Christiansen effect. This effect is caused by a refraction index mismatch between the salt (KBr) and the sample powder that leads to reflections at the salt-sample interface. Therefore, proper grinding is required to ensure a good contact between KBr and sample powder and to minimize the portion of the reflected light.

Another important factor in this technique is to keep everything moisture free as the KBr material is hygroscopic. To prevent the KBr material from absorbing moisture, keep the KBr material and the die in a drying oven at a temperature of 50 to 60°C. Failure to do so will result in opaque pellets that yield distorted spectra. A correctly prepared KBr pellet will be transparent to IR light.

To sum it up, the KBr-pellet technique yields good quality spectra with a wide spectral range and no interfering peaks. Disadvantages include tedious and time consuming sample preparation and cleanup, interference of water bands (3,960 to 3,480cm^{-1} and 1,950 to 1,300cm^{-1} and below 500cm^{-1}) and in same cases structural changes caused by high pressure applied to the KBr/sample mix.

- Put a small amount of the sample in an agate mortar and grind it up as fine as possible.
- Add a spatula of oven-dry KBr material to the ground sample and mix it until a uniform mixture is obtained. Do not grind the mixture as this may increase the absorption of water by KBr.

➢ A common mistake is to use to much sample. The concentration of the sample in KBr should be in the range of 0.2% to 1% (i.e. typically a 300:1 dilution by mass).

- Transfer the mixture into a die of a hydraulic or hand press and subject it to very high pressure (ca. 20,000 psi) for a few minutes (2 to 5 minutes). The result should be a translucent pellet with an ideal thickness of 0.5 to 1mm.
- Carefully remove the pellet from the die, place it in the pellet holder and put the pellet holder in the spectrometer sample compartment.

➢ The KBr pellet is very hygroscopic and fragile. Handle it with care and use gloves to avoid contact with moisture from your hands. Measure the KBr pellet immediately after removing it from the press as the pellet will fairly rapidly begin to absorb moisture from the air and becomes opaque.

F.2.6 Liquid cell

Liquid cells produce excellent results for most liquids. Especially for liquid samples that are very volatile, using a liquid cell is highly recommended. A liquid cell consists of two IR transparent windows with a precision spacer in between. One of the windows has two drilled holes for the introduction and evacuation of the liquid. A large number of cell options are available including permanently sealed cells, demountable cells with different window material and a wide selection of spacers.

➢ Take into consideration that KBr is hygroscopic and the pathlength of the KBr cell will change when exposed to a ‘wet’ sample (this may affect quantitative results). In addition, water will reduce the cell throughput by clouding the windows. Note that many liquid cells contribute a fringe pattern to the spectrum. Matching the refraction index of the window material with that of the sample can minimize this effect.

F.2.7 Gas cell

To obtain an infrared spectrum of a gaseous sample a gas cell with windows at each end is required. It is important to select a suitable window material (e.g. KBr, NaCl, or CaF_2) that does not absorb infrared light. The cell usually has an inlet and outlet port with a tap to facilitate the filling with the gas to be analyzed. Simple demountable cells (50 mm to 100 mm) are recommended for samples in a 5 - 10% concentration range. For diluted samples (ppm to ppb concentrations) a long path cell should be used. The long path cell reflects the IR beam several times through the sample using a set of mirrors positioned on the opposite ends of the cell. Note that the cell thickness, the pressure of the gas (proportional to concentration) inside the cell, and the molar absorptivity determine the peak intensity.

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