



INVENIO R

User Manual

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© 2019 BRUKER OPTIK GmbH, Rudolf-Plank-Straße 27
D-76275 Ettlingen, www.bruker.com

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This manual is the original documentation for the FT-IR spectrometer INVENIO R. 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

	<ul style="list-style-type: none">➤ 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 and operated as well as maintained and repaired according to the procedures described in this manual and in compliance with all relevant safety standards and regulation.➤ The spectrometer should be operated only by authorized personnel which is trained in operating the spectrometer and which is familiar with the relevant safety instructions and laser safety regulations.➤ 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.
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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
	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, KRS-5)
	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, BaF ₂)

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:

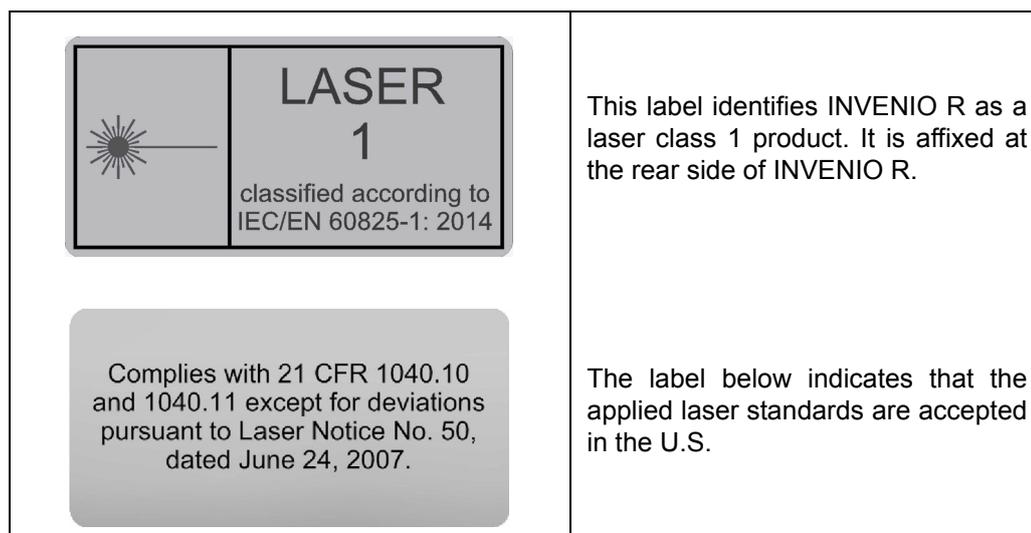
Symbol	Definition
	<p>Infectious material</p> <p>This warning symbol indicates the possible existence of biologically dangerous and infectious material. When working with this kind of material always observe the prevailing laboratory safety regulations and take necessary precautions and disinfection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

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 R 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.



The spectrometer is equipped with a HeNe laser. This laser emits red light with a wavelength of 633 nm. The rated cw optical power output is 0.8 mW. According to EN 60825-1, the incorporated laser is laser class 2 product.

Under normal circumstances, radiation of a laser class 2 laser does not pose a health hazard. Nonetheless, do avoid any exposure to the laser beam and do not stare into the laser beam.

1.5 Intended use

INVENIO R 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

➤ **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 R is characterized by the following technical key features:

Innovative detector technology

By default, the spectrometer has a multi-detector unit which can accommodate up to five detectors such as DTGS, InGaAs, Si diode and GaP. These detectors do not require additional cooling with liquid nitrogen. With the multi-detector unit, the entire spectral range from FIR to UV/VIS can be covered without the need for exchanging the detector. The detectors are software selectable. The signal is digitized directly in place by a dual-channel A/D converter with a 24-bit dynamic range.

Optionally, the spectrometer can be equipped with an additional detector position for installing a DigiTect-type detector (e.g. MCT, DTGS). The DigiTect detectors are equipped with an integrated preamplifier and an A/D converter with 24-bit dynamic range which 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 ensures a high signal-to-noise-ratio.

All these detectors are available for measurements with the large-sized sample compartment only. Additionally, the DigiTect-type detector position can be used for emission measurements bypassing the sample compartment.

☞ For detailed information about the available detectors, see section 4.5.3.

Possibility for extending the spectral range and automatic component recognition (ACR)

The standard spectrometer configuration is equipped for data acquisition in the mid IR region (8,000 to 350 cm^{-1}). Optionally, the spectrometer can be equipped with different optical components to cover the spectral range from the far infrared range (15 cm^{-1}) up to the ultraviolet range (28,000 cm^{-1}). In this context, the optionally available ultra-wide range beamsplitter and the wide range DTGS detector are special key features. In combination with the standard internal IR source, these components cover the complete far and mid IR range (6,000 cm^{-1} to 80 cm^{-1}) without the need for any component exchange.

☞ For information about the available spectral range packages, see section 2.2.

The function ACR recognizes automatically the currently installed optical components like source, detector, beamsplitter and windows (e.g. sample compartment windows). These components are electronically coded so that the spectrometer firmware can 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 spectrometer components are monitored permanently to ensure that they operate within the specification range. This feature is called Performance Guard. Its purpose is to facilitate fault diagnostics and maintenance.

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 R&D 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.

Automatic accessory recognition (AAR)

The function AAR identifies automatically the QuickLock-type accessory currently installed in the large-sized sample compartment, performs several tests and loads automatically the corresponding experiment file including the pre-defined measurement parameters. It facilitates performing spectroscopic measurements and ensure reliable measurement results.

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 R&D tasks by simplified work-flows and intuitive operation.

2.2 Available spectral range packages

The spectral range in which the spectrometer is capable of detecting a signal is determined by the following optical spectrometer components:

- source
- beamsplitter
- detector
- sample compartment window

There are predefined spectrometer configurations which allow for certain spectral ranges. The following spectral range packages are available:

1) Standard spectral range: MIR 8,000 to 350 cm⁻¹

Optical component	This spectral range package includes:
Source	MIR source (installed internally)
Beamsplitter	KBr beamsplitter
Detector	DTGS with KBr window
Sample compartment is equipped with:	KBr windows

2) Extended spectral range: MIR + FIR 6,000 to 130 cm⁻¹

Optical component	This spectral range package includes:
Source	MIR source (installed internally)
Beamsplitter	wide range beamsplitter for mid-IR and far-IR range
Detector	DTGS with CsI window
Sample compartment is equipped with:	automatic shutters

3) Extended spectral range: MIR + FIR 6,000 to 80 cm⁻¹

Optical component	This spectral range package includes:
Source	MIR source (installed internally)
Beamsplitter	wide range beamsplitter for mid-IR and far-IR range
Detector	wide range DTGS
Sample compartment is equipped with:	automatic shutters

4) Extended spectral range: MIR + FIR 6,000 to 15 cm⁻¹

Optical component	This spectral range package includes:
Source	2x sources <ul style="list-style-type: none"> • MIR source (globar, installed internally) • FIR source (Hg lamp, installed externally)
Beamsplitter	wide range beamsplitter for mid-IR and far-IR range
Detector	Multi detector unit with two detectors: <ul style="list-style-type: none"> • DTGS-CsI detector (for MIR) • DTGS-PE detector (for FIR)
Sample compartment is equipped with:	automatic shutters

5) Extended spectral range: MIR + NIR/VIS 15,500 to 350 cm⁻¹

Optical component	This spectral range package includes:
Source	2x sources: <ul style="list-style-type: none"> • MIR source (globar, installed internally) • NIR source (Halogen lamp, installed internally)
Beamsplitter	2x beamsplitters: <ul style="list-style-type: none"> • KBr beamsplitter (for MIR) • CaF₂ beamsplitter (for NIR/VIS) Note: Depending on the intended spectral range, the corresponding beamsplitter has to be installed. See section 5.10.
Detector	Multi detector unit with two detectors: <ul style="list-style-type: none"> • DTGS-KBr detector (for MIR) • InGaAs diode (for NIR)
Sample compartment is equipped with:	KBr windows

6) Extended spectral range: MIR + NIR + VIS 25,000 to 350 cm⁻¹

Optical component	This spectral range package includes:
Source	2x sources: <ul style="list-style-type: none"> • MIR source (globar, installed internally) • NIR source (Halogen lamp, installed internally)
Beamsplitter	2x beamsplitters: <ul style="list-style-type: none"> • KBr beamsplitter (for MIR) • Quartz beamsplitter (for NIR/VIS) Note: Depending on the intended spectral range, the corresponding beamsplitter has to be installed. See section 5.10.
Detector	Multi detector unit with three detectors: <ul style="list-style-type: none"> • DTGS-KBr detector (for MIR) • InGaAs diode (for NIR) • Si diode (for VIS/UV)
Sample compartment is equipped with:	2 types of window: <ul style="list-style-type: none"> • KBr windows (for MIR) • CaF₂ windows (for NIR & VIS) Note: Depending on the intended spectral range, the corresponding type of window has to be installed. See section 5.12.

7) Extended spectral range: FIR + MIR + NIR + VIS 25,000 to 30 cm⁻¹

Optical component	This spectral range package includes:
Source	2x sources: <ul style="list-style-type: none"> • MIR source (global, installed internally) • NIR source (Halogen lamp, installed internally)
Beamsplitter	3x beamsplitters: <ul style="list-style-type: none"> • KBr beamsplitter (for MIR) • Quartz beamsplitter (for NIR/VIS/UV) • Solid state beamsplitter (for FIR) Note: Depending on the intended spectral range, the corresponding beamsplitter has to be installed. See section 5.10.
Detector	Multi detector unit with four detectors: <ul style="list-style-type: none"> • DTGS-KBr detector (for MIR) • InGaAs diode (for NIR) • Si diode (for VIS & UV) • DTGS-PE (for FIR)
Sample compartment is equipped with:	either windows or automatic shutters 3 types of windows: <ul style="list-style-type: none"> • KBr window (for MIR) • CaF₂ window (for NIR/VIS/UV) • PE window (for FIR) Note: Depending on the intended spectral range, the corresponding type of window has to be installed. See section 5.12.

8) Extended spectral range: MIR + NIR + VIS/UV 28,000 to 350 cm⁻¹

Optical component	This spectral range package includes:
Source	3x sources: <ul style="list-style-type: none"> • MIR source (global, installed internally) • NIR source (Halogen lamp, installed internally) • VIS/NIR source (Halogen lamp, installed externally)
Beamsplitter	2x beamsplitters: <ul style="list-style-type: none"> • KBr beamsplitter (for MIR) • Quartz beamsplitter (for NIR/VIS/UV)

Optical component	This spectral range package includes:
Detector	Multi detector unit with four detectors: <ul style="list-style-type: none"> • DTGS-KBr detector (for MIR) • InGaAs diode (for NIR) • Si diode (for VIS/UV) • GaP diode (for VIS/UV)
Sample compartment is equipped with:	either windows or automatic shutters 3 types of windows: <ul style="list-style-type: none"> • KBr window (for MIR) • CaF₂ window (for NIR/VIS/UV) or • Quartz window (for NIR/VIS/UV) <p>Note: Depending on the intended spectral range, the corresponding type of window has to be installed. See section 5.12.</p>

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 being equipped with different standards (test samples) used for validating and testing the instrument performance. Depending on which test protocol (OQ¹ or PQ²) 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 OVP³.

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

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

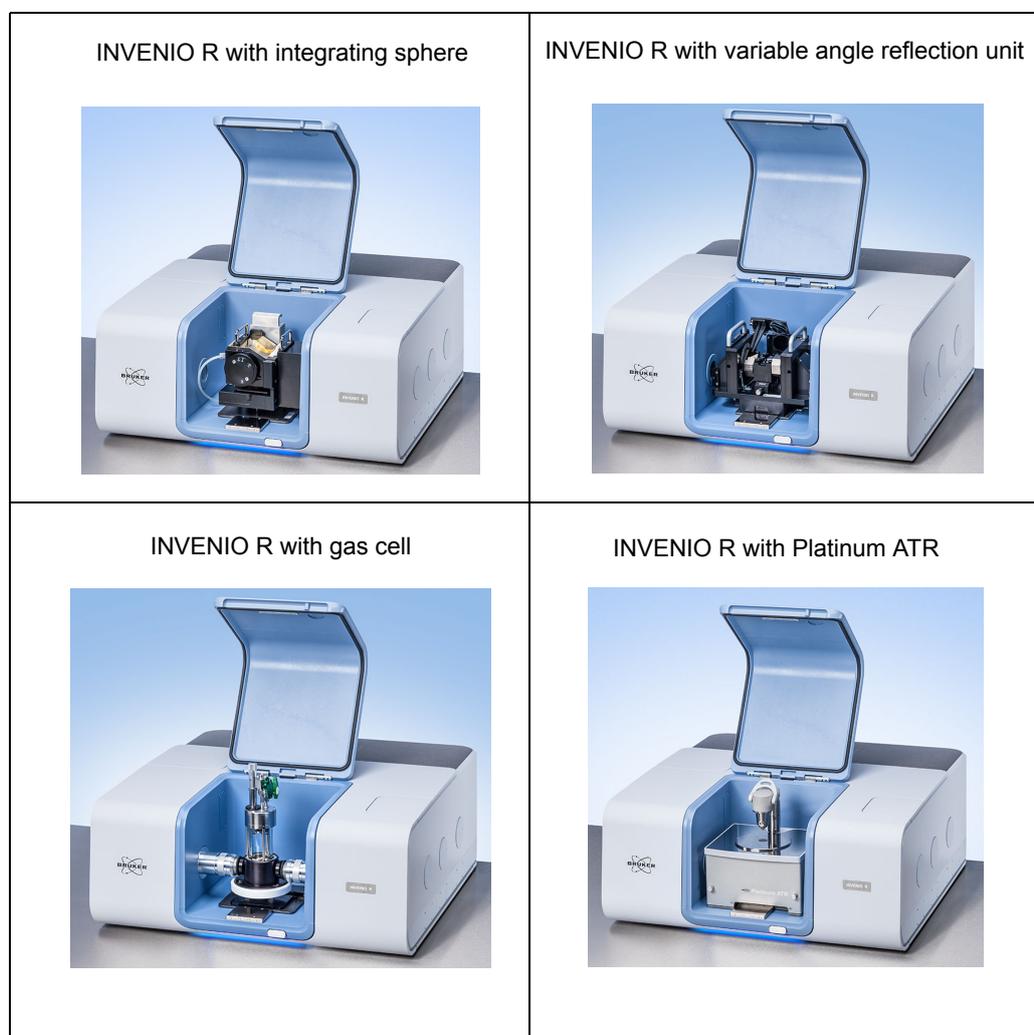


Figure 2.1: INVENIO R with different QuickLock-type accessories installed in the large-sized sample compartment

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 (on the right and left side) and two IR beam inlet ports (on the right and rear side) allowing the connection of a multitude of optional accessories and/or components like:

- coupling of TGA¹ and GC² instruments
- PMA 50 (Polarization Modulation Accessory for applications in the field of VCD³ and PM-IRRAS⁴)
- HYPERION 1000/2000 IR microscope and HYPERION 3000 imaging microscope with FPA detector (Focal Plane Array detector system)
- IMAC module (Imaging Accessory with FPA detector)
- HTS-XT module (High Throughput Screening Extension)
- PL II module (Photo luminescence module)
- Fiber optic coupling module with MIR or NIR fiber probes for solid and liquid samples
- FT Raman module (e.g. RAM II)
- FIR bolometer
- Externally connected, Hg-arc source

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

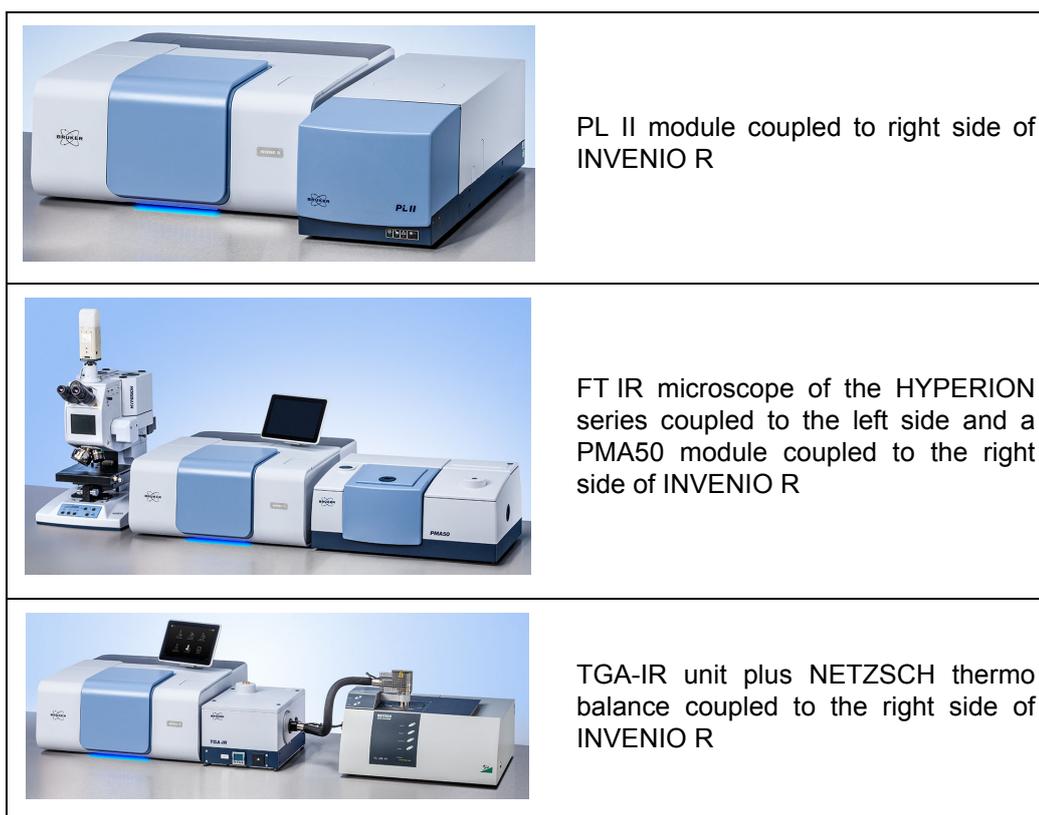


Figure 2.2: Examples of possible instrumental set-ups

1. TGA - Thermogravimetric Analysis
2. GC - Gas Chromatography
3. VCD - Vibrational Circular Dichroism
4. PM-IRRAS - Polarization Modulation Infrared Reflection Absorption Spectroscopy

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 R* 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 delivered items are divided into standard components and optional components. So the actual delivery scope depends on the customer's order.

Standard components:	The standard delivery scope includes the following items: <ul style="list-style-type: none">• INVENIO R (including the user manual)• External power supply unit with low-voltage cable, power cord• PC compatible data system (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.)• OPUS software, basic IR package (including the OPUS Reference Manual)
Optional components:	The delivery scope can also include following optional components: <ul style="list-style-type: none">• Optional spectrometer components (e.g. optional detectors, sources and/or beamsplitter)• Optional accessories• Panel PC with installed OPUS/TOUCH software• Optional OPUS software packages (QUANT, IDENT, etc.) including the corresponding manuals• Purge option S316/7 (Note: This option includes the required hoses and an air flow regulator.)

3.3 Inspecting the packaging

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



CAUTION

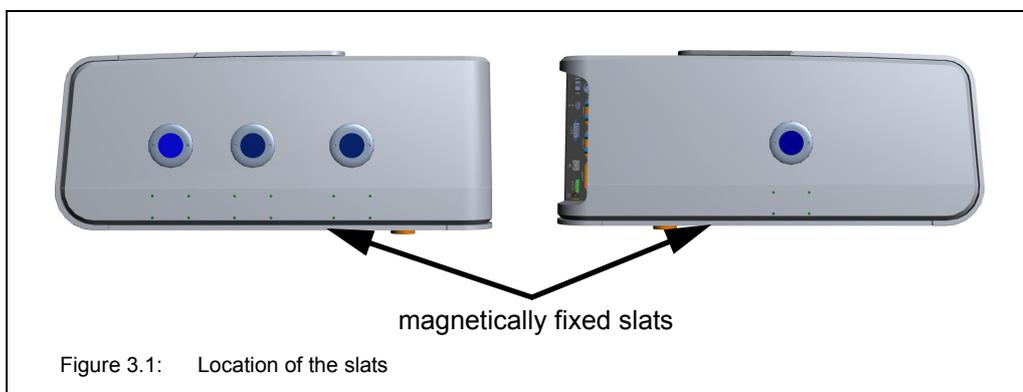
Possible damage to the delivered spectrometer because of transport damage

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!**



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:	<ul style="list-style-type: none"> • 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:	<ul style="list-style-type: none"> • 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:	<ul style="list-style-type: none"> • 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. <p>Note: The local purge gas supply line needs to be dimensioned for a PVC hose having an outer diameter of 6 mm.</p> <hr/> <p>i For regulating the purge gas flow rate, an air flow regulator (order no: S316/7) is optional available.</p> <hr/>

<p>Power supply requirements:</p>	<p>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.</p> <ul style="list-style-type: none"> • Input range: 100 - 240 V AC, 50 - 60 Hz • Output: 24 V DC, 5 A <p>Connect the spectrometer only to a socket outlet with earthing contact that complies with VDE 0620-1 or IEC!</p> <p>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.</p> <p>If there are problems concerning main power supply (e.g. brownouts, power surges, frequent thunderstorms or power blackouts) use an UPS unit (<u>U</u>ninterruptible <u>P</u>ower <u>S</u>upply) to ensure an uninterruptible power supply and consequently an operation without interruptions.</p>
<p>Possibilities of interrupting the mains power supply:</p>	<p>The mains power supply of the spectrometer can be interrupted as follows:</p> <ul style="list-style-type: none"> • by pulling the mains plug of the power cord • by pulling the power cord from the external power supply unit • by switching off the spectrometer using the ON / OFF switch at the spectrometer rear side
<p>External devices:</p>	<ul style="list-style-type: none"> • 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 (<u>s</u>afety <u>e</u>xtra <u>l</u>ow <u>v</u>oltage circuit). <hr/> <p>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).</p> <hr/>

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, 50 - 60 Hz
- Output: 24 V DC, 5 A

i 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

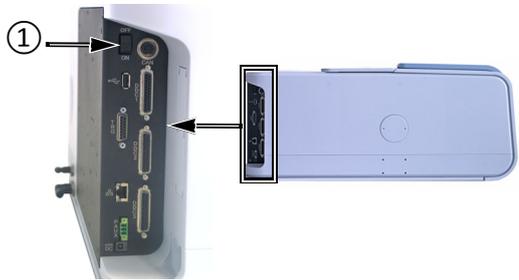
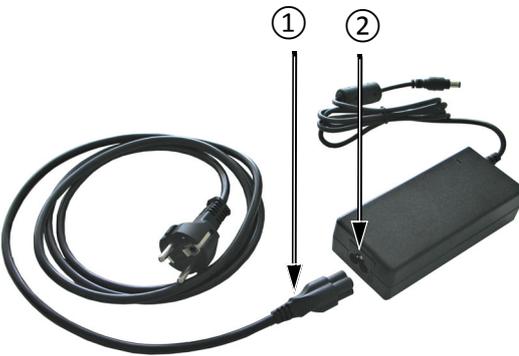
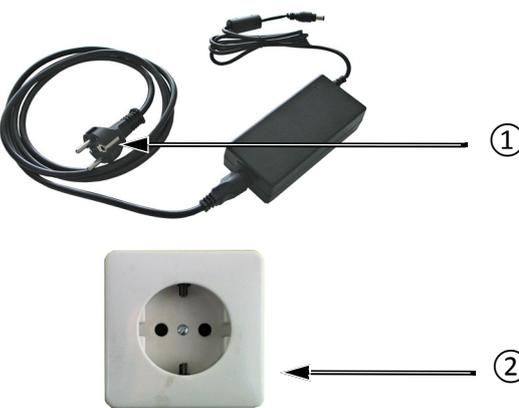
Electric shock hazard because of power supply unit damage or unauthorized repair

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		<p>Make sure that the spectrometer is switched off. To do this, check the setting of the ON/OFF switch ①.</p>
2		<p>Connect the power cord ① to the C5 connector of the external power supply unit ②.</p>
3		<p>Connect the low-voltage cable ① to the low-voltage socket ② at the spectrometer rear side.</p>
4		<p>Connect the power plug ① of the power cord to the mains socket outlet ②.</p> <p>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!</p>

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.

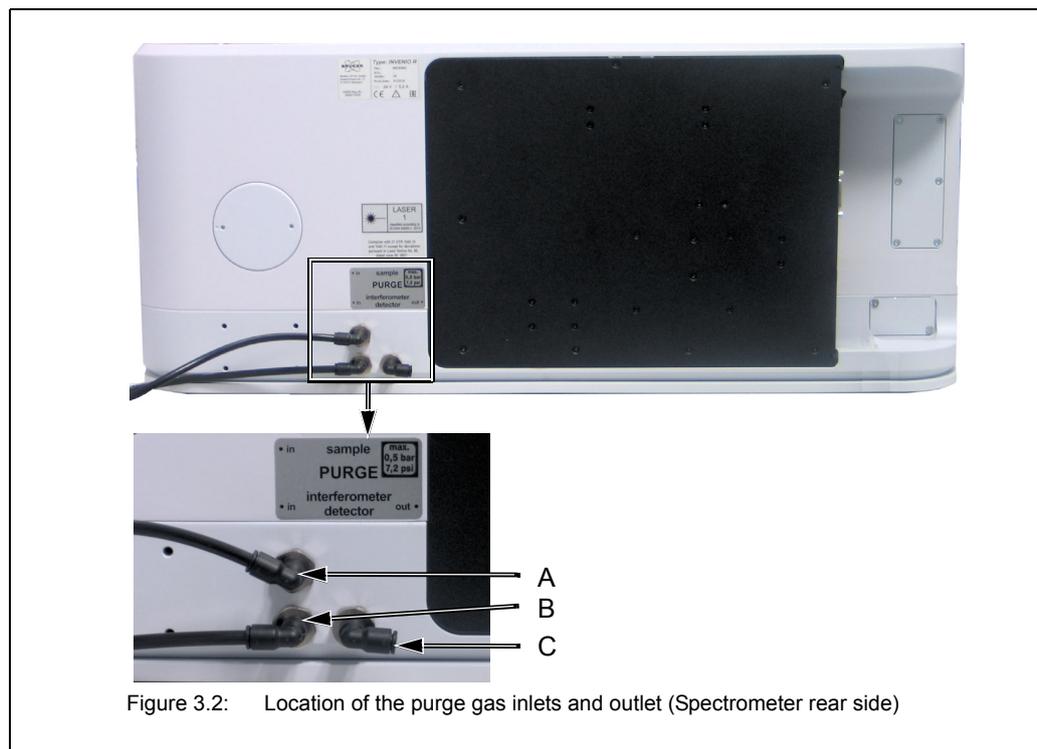


Figure 3.2: Location of the purge gas inlets and outlet (Spectrometer rear side)

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

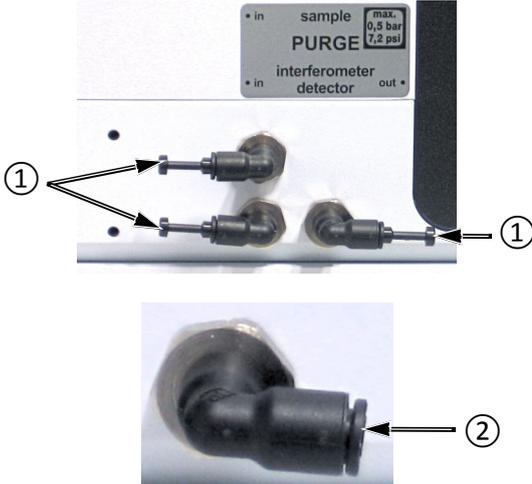
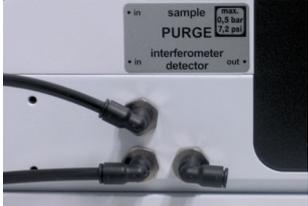
3.7.2 Purge gas supply requirements

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 overpressure)
- 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

- i** 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: 6 mm). 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.

1		<p>Remove the plugs ① from the purge gas inlets and the purge gas outlet.</p> <p>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.</p> <p>To remove a plug, press the lock ring ② inwards and pull out the plug.</p> <p>Note: All purge gas ports have such a lock ring. The lock ring prevents the hose from being pulled out unintentionally.</p>
2		<p>Insert the hoses into the purge gas inlets.</p>
4	<p>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).</p>	

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.
- In case the optical bench is purge, remove the plug from the purge gas outlet as well.
- Connect the other end of the hose to the local purge gas supply line.

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.

	<p>INVENIO R 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.</p>
	<p>INVENIO R 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.</p> <p>☞ For information about the possible connection variants and the installation procedures, see sections 3.8.2.</p>
	<p>INVENIO R 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.</p> <p>☞ For information about the possible connection variants and the installation procedures, see sections 3.8.3.</p>
	<p>INVENIO R connected to a tablet PC</p> <p>☞ For information about the installation procedure, see section 3.8.4.</p>

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 ***

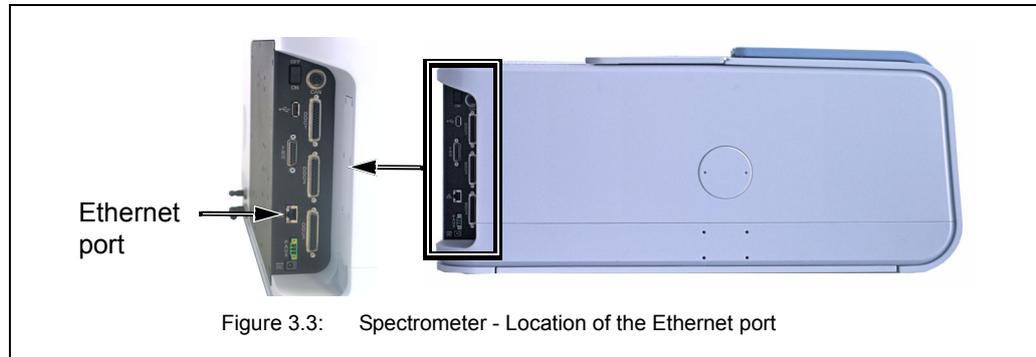
Note: Normally, PC, laptop and/or tablet are delivered by Bruker. If desired, they can also be provided by the operating company.

* 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).



Depending on the connection variant, the data cable is connected to different Ethernet ports at the PC. (For information about possible connection variants, see section 3.8.2.)

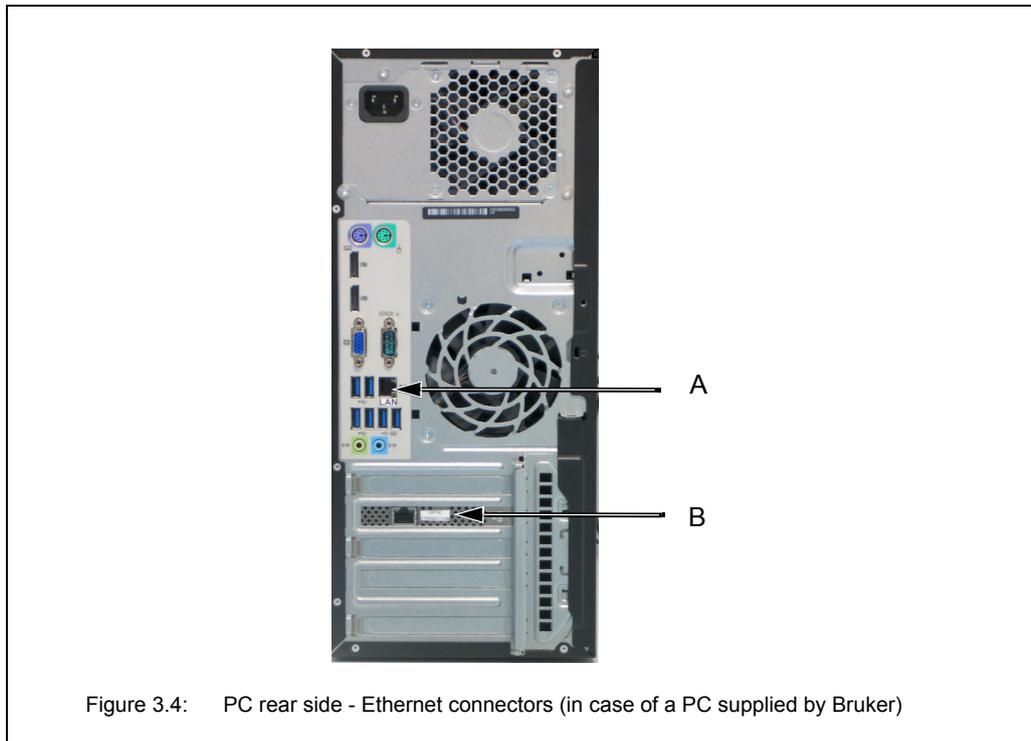
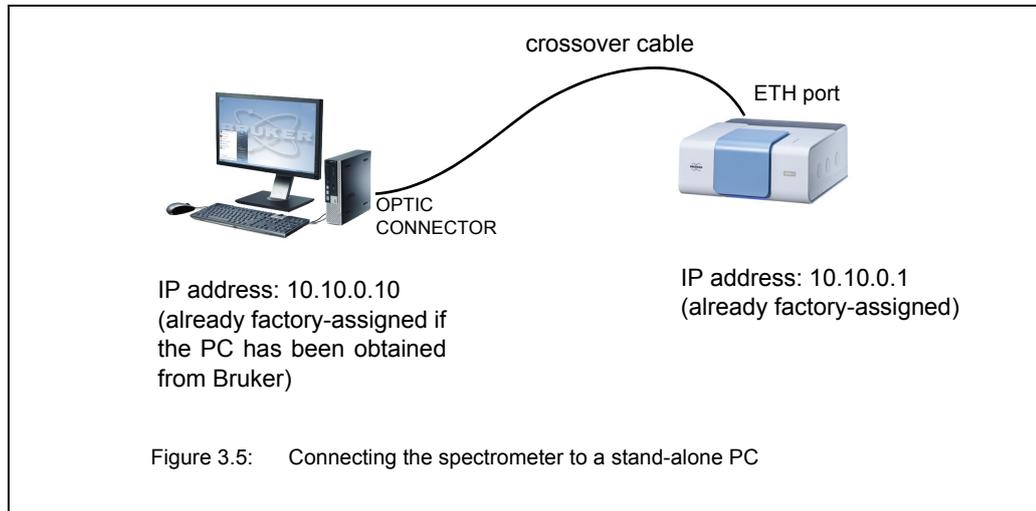


Fig. 3.4	Ethernet port
A	labeled LAN Note: At this Ethernet port, connect only a straight through data cable.
B	labeled OPTIC CONNECTOR Note: At this Ethernet port, connect only a crossover data cable.

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

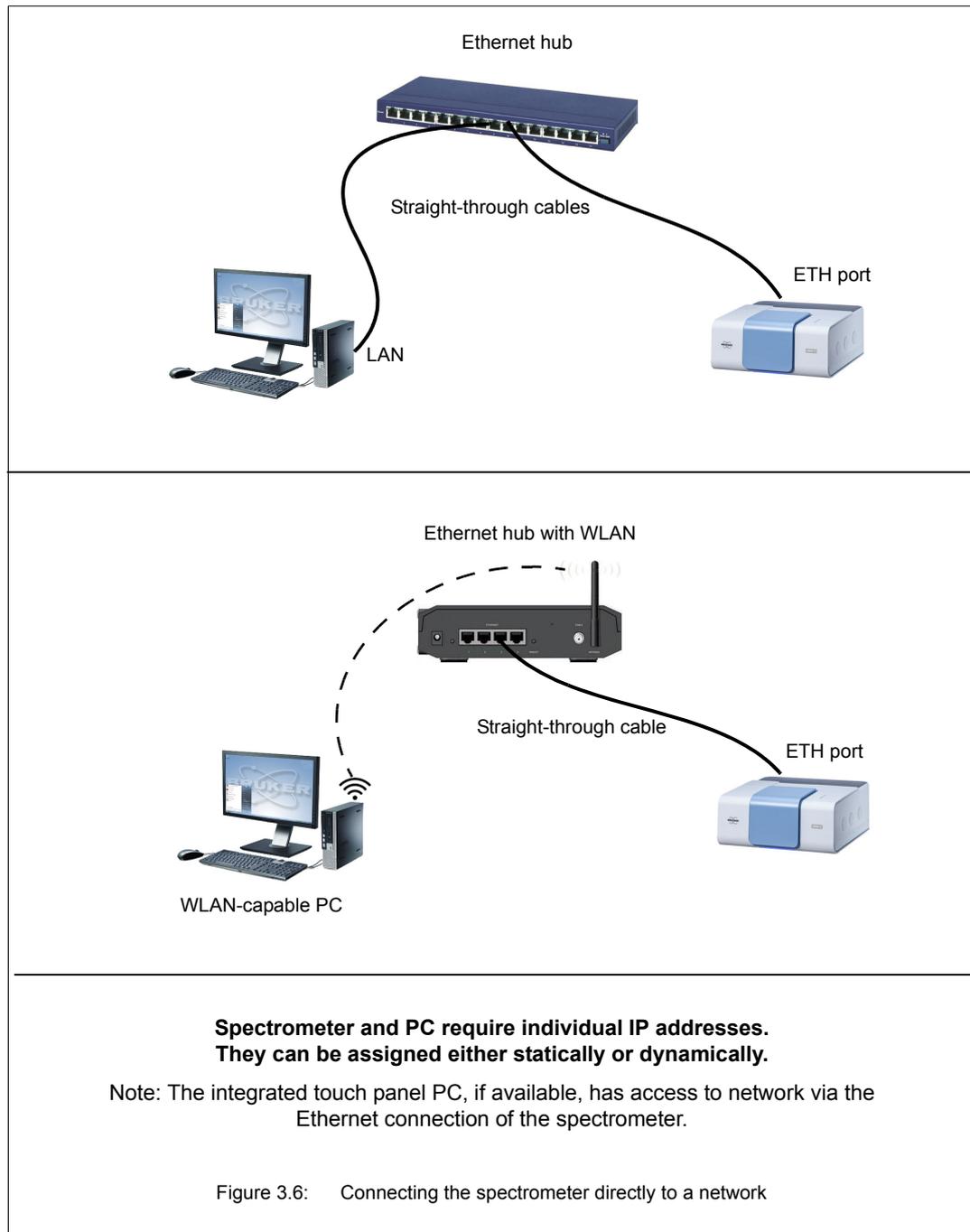


Procedure

- 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 CONNECTOR¹ (B in fig. 3.4) at the PC rear side.
- 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.
- 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



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 LAN¹ 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).

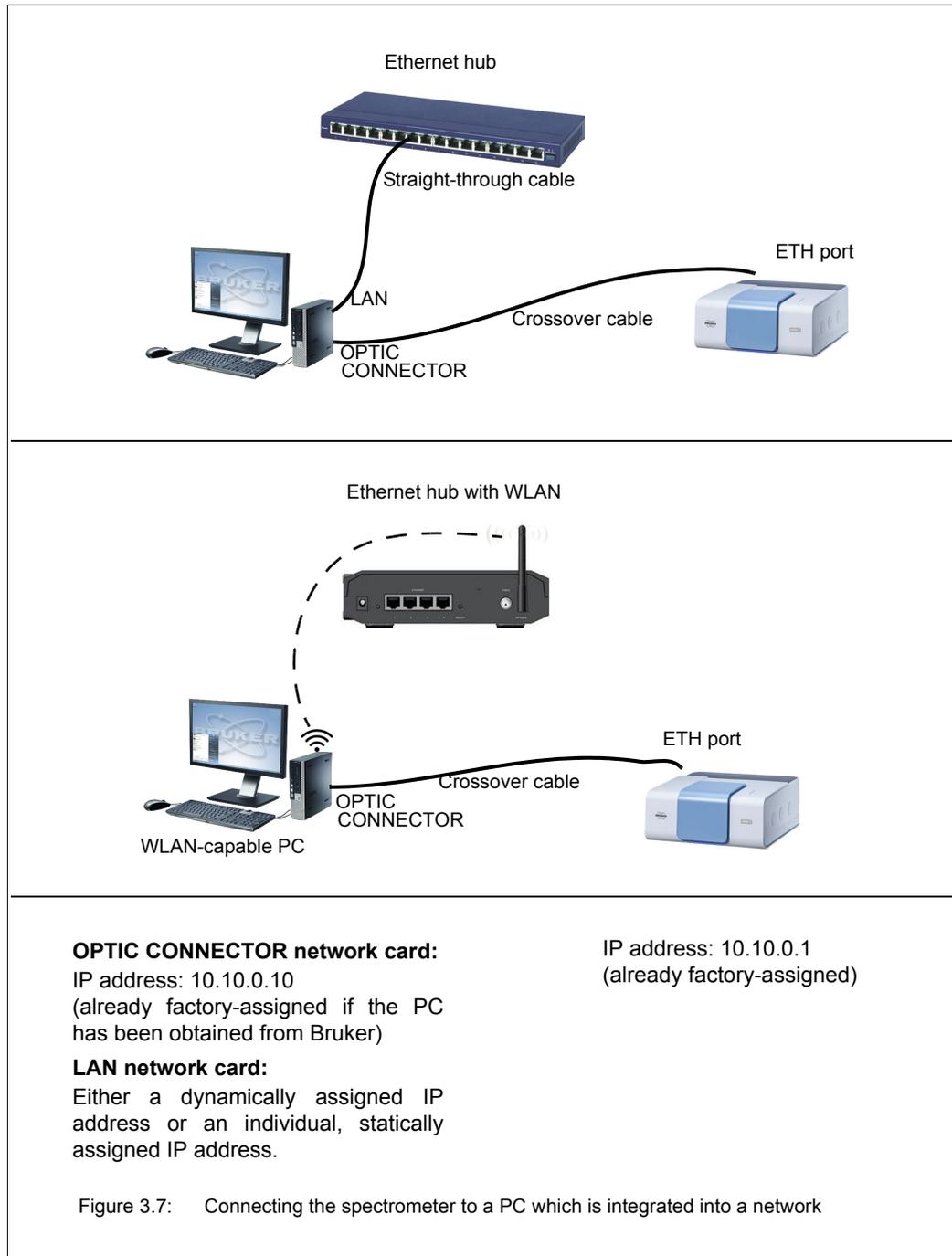
3. IP address assignment

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.

Variation C: Connecting the spectrometer to a network PC



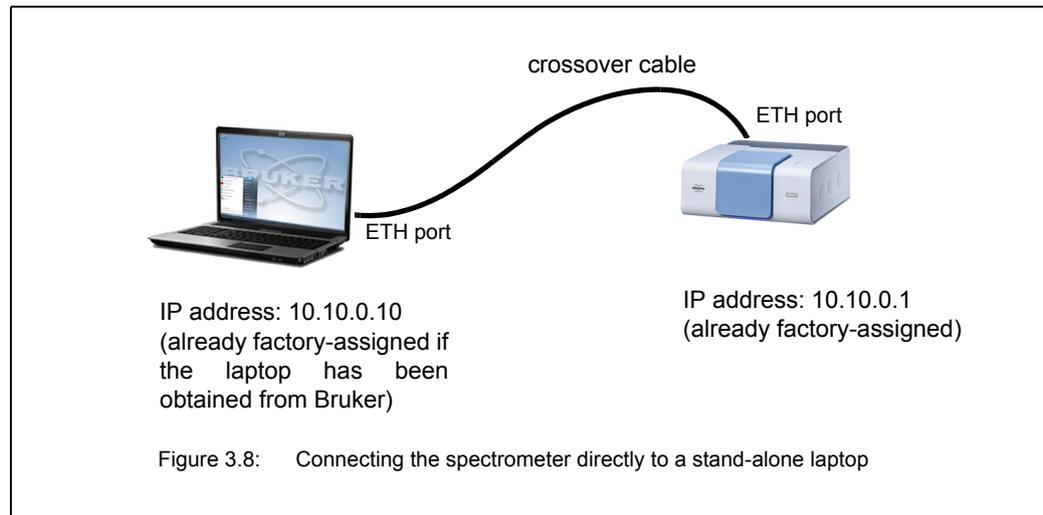
Procedure

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 CONNECTOR¹ (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 LAN¹ connector (A fig. 3.4) at the PC rear side and to a 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

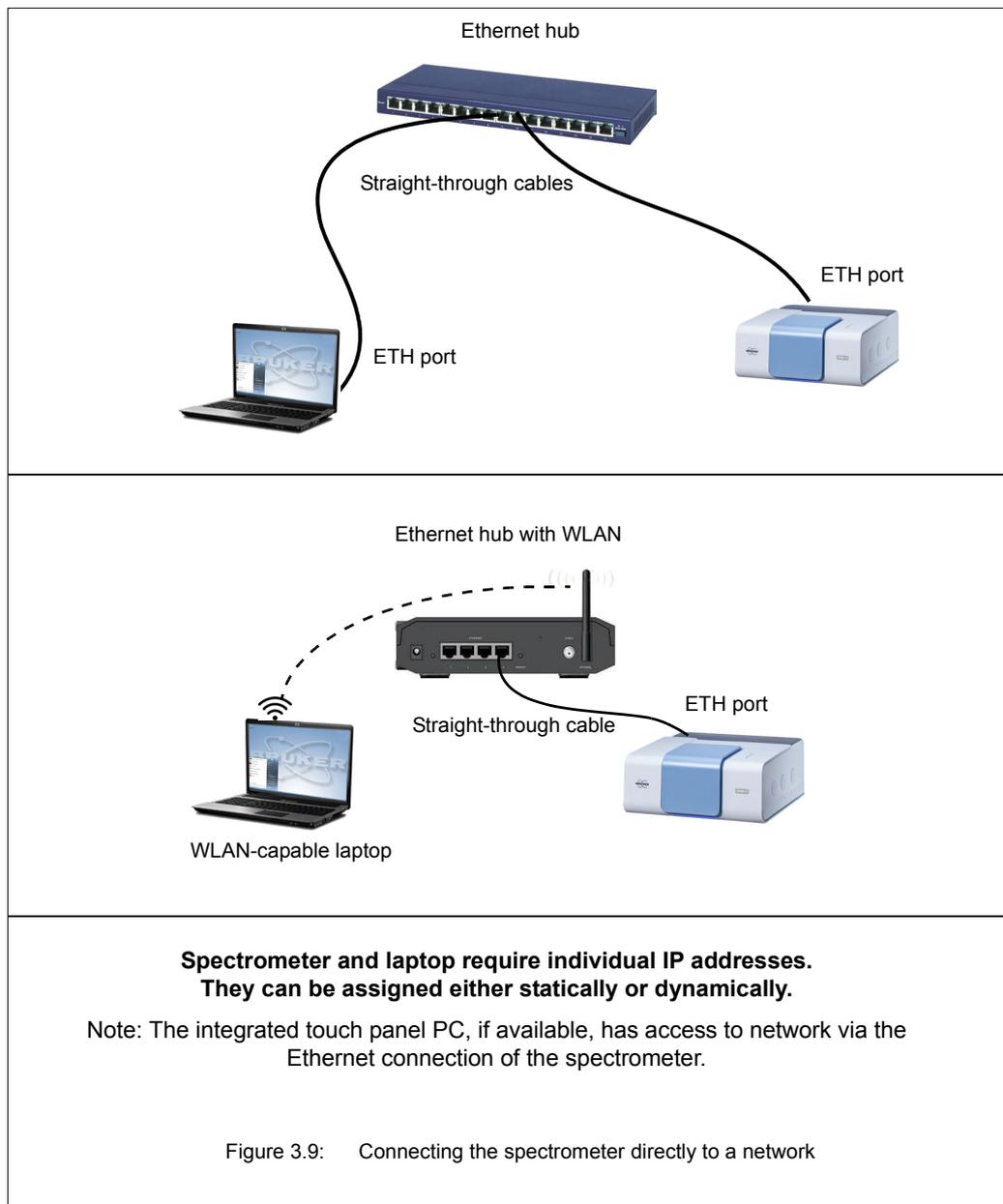
Variant A: Connecting the spectrometer to a stand-alone laptop



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.)

Variation B: Connecting both spectrometer and laptops 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

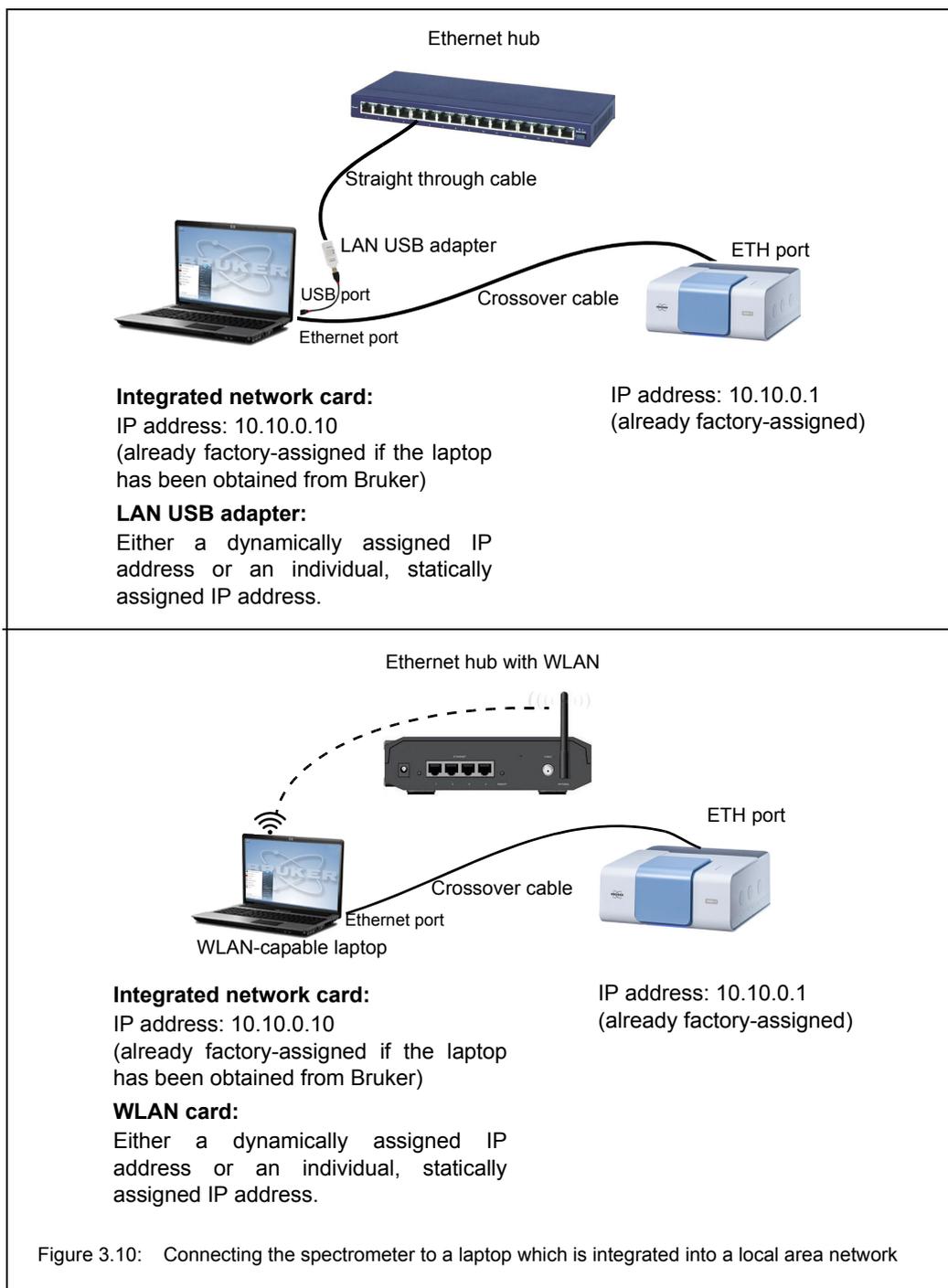
All IP addresses (i.e. IP address of the spectrometer and the laptop) can be assigned either dynamically or statically. In the latter case, your network administrator has to define the static IP addresses.

- 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.

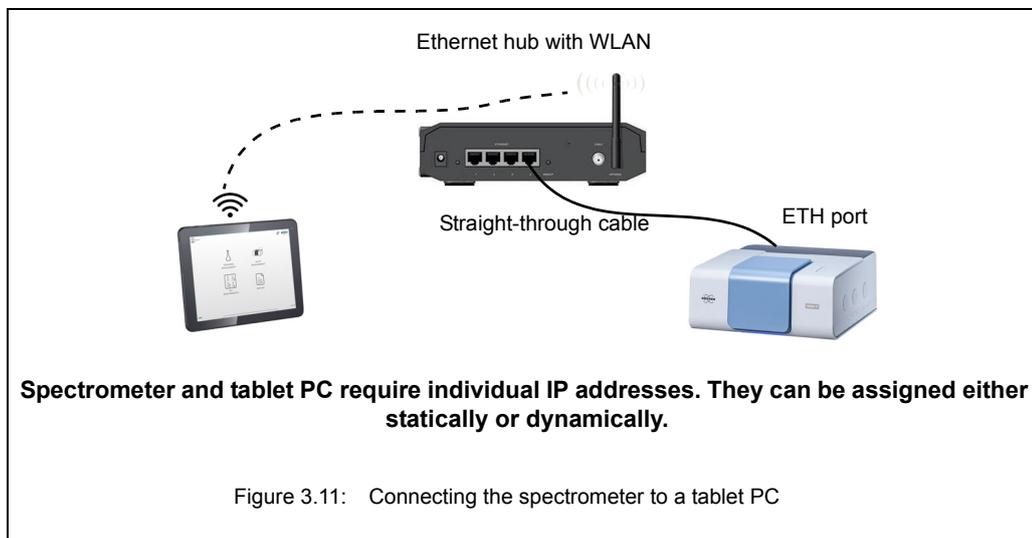


Procedure

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



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 (factory-configured variant):

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	255.255.255.240	255.255.255.0	--
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:

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 a 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:

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	255.255.255.240	255.255.255.0	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.

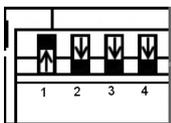
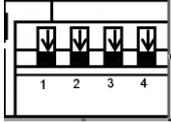
	Spectrometer	network card installed in the PC	LAN USB adapter
IP address	10.10.0.1	10.10.0.10	defined by network administrator or DHCP
Subnet mask	255.255.255.240	255.255.255.0	defined by network administrator
Gateway	0.0.0.0 Do not define in case of Windows XP.	0.0.0.0 Do not define in case of Windows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

3.8.6 Assigning an IP address to the spectrometer

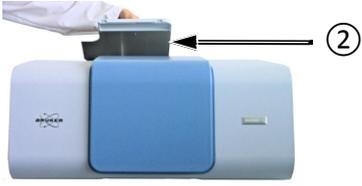
3.8.6.1 General information

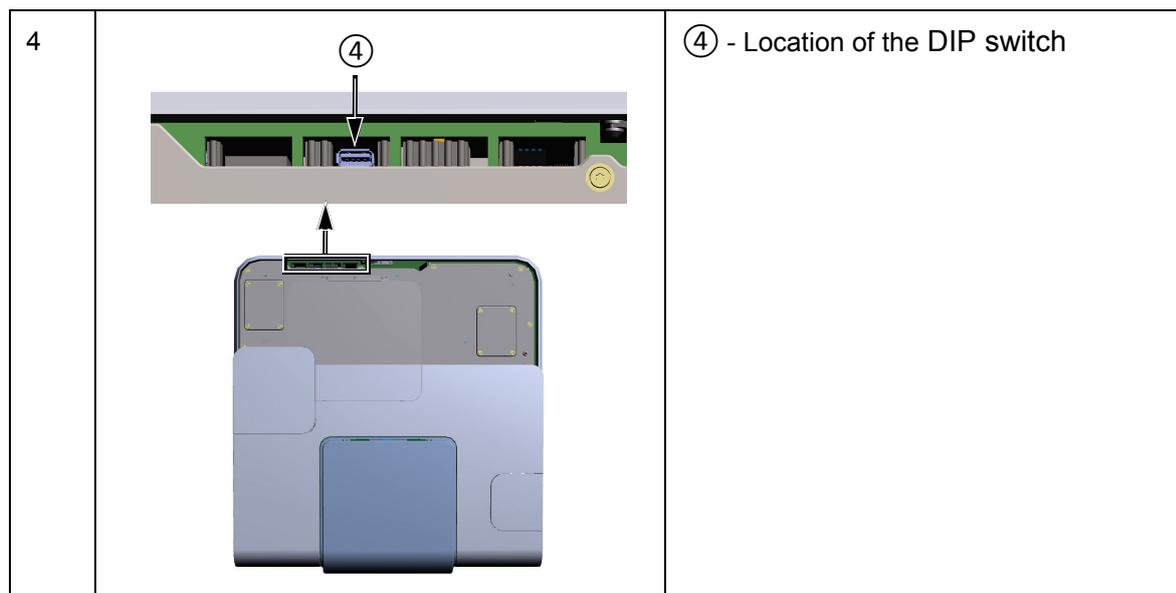
By default, the spectrometer is delivered with the factory-assigned standard IP address 10.10.0.1. In case of connection variant A and C, there is no need for assigning a different IP address to the spectrometer. Only in case of connection variant B (i.e. connecting the spectrometer directly to a network, 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:

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

How to get access to the spectrometer DIP switch

<p>1</p>		<p>1. Remove the plastic cover (1) which provides access to the DigiTect detector.</p> <p>Note: This cover is held in place magnetically.</p>
<p>2</p>		<p>2. Fold back the outer lid (2) to facilitate the removal of the metallic cover.</p>
<p>3</p>		<p>3. Remove the metallic cover (3).</p>



3.8.6.2 IP address assignment by DHCP

General Information

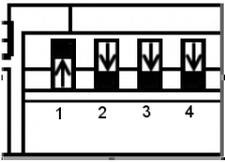
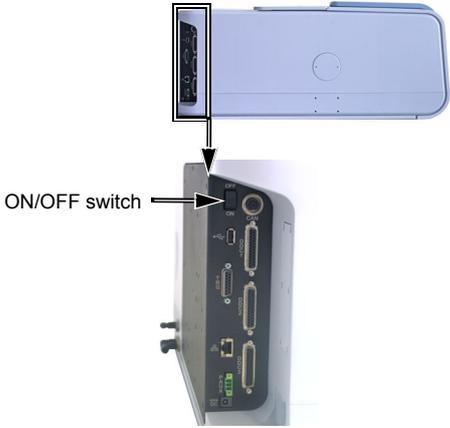
- A DHCP¹-based IP address assignment requires a DHCP server integrated into the local network.

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.

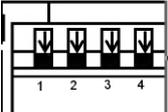
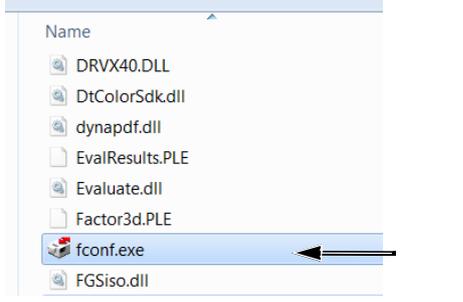
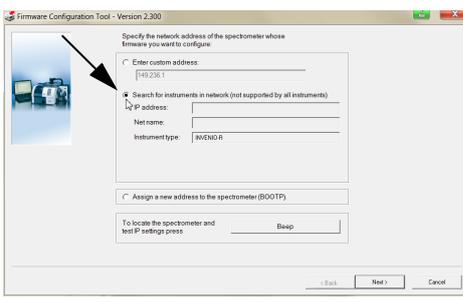
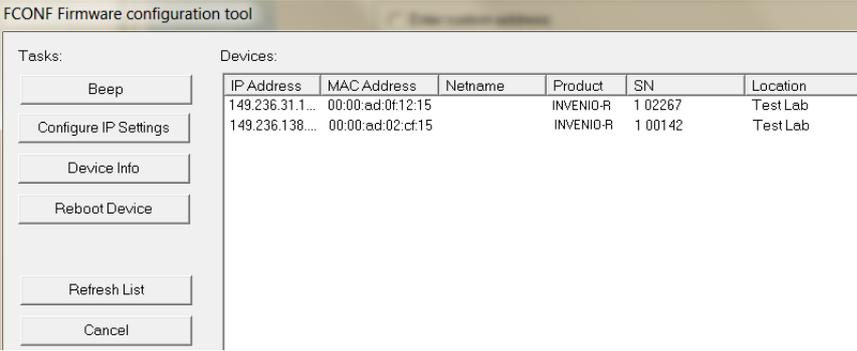
1. DHCP (Dynamic Host Configuration Protocol) is a protocol that automatically assigns IP addresses to the devices connected in a network. If several devices (e.g. PCs, spectrometers etc.) are connected to a local network simultaneously, the DHCP server assigns a unique IP address to each device. Possible 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.

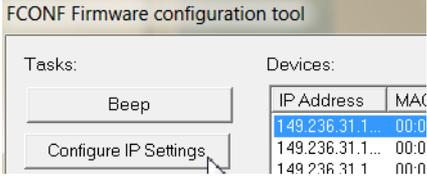
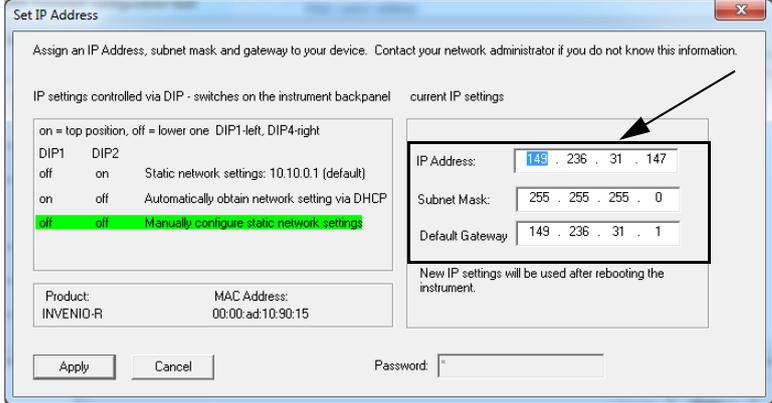
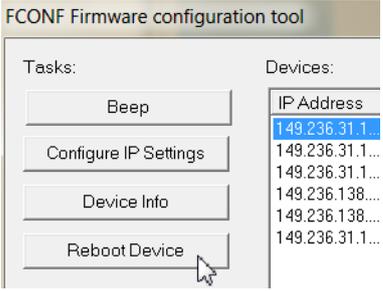
Procedure

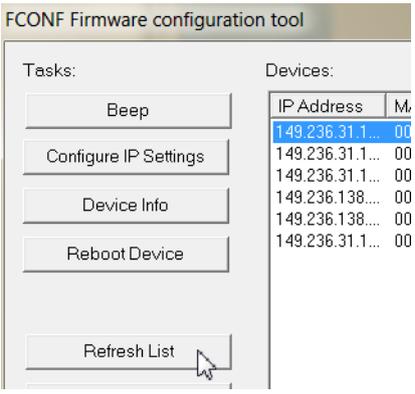
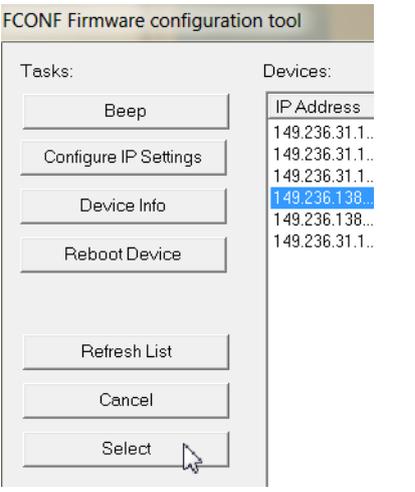
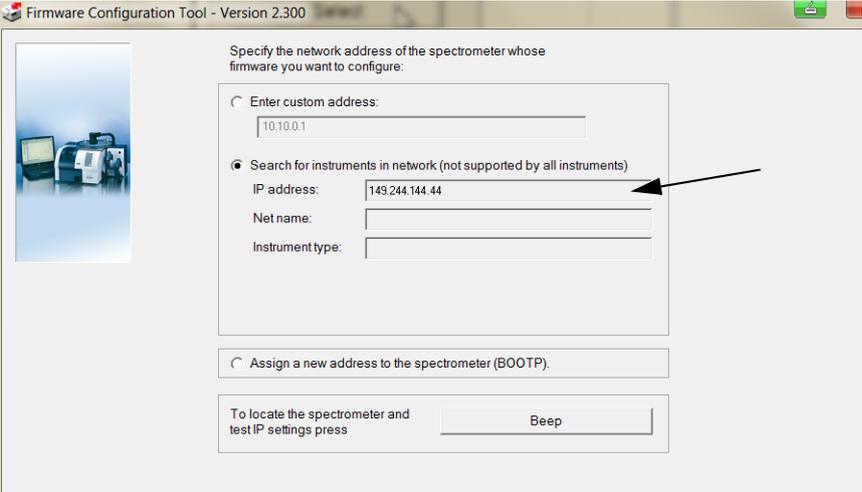
1	<p>Only in case of static DHCP: On the DHCP server, the network administrator has to set up a DHCP reservation (i.e. a certain IP address) for the spectrometer in question (on the basis of the spectrometer MAC address).</p>	
2		<p>Check whether the first DIP switch is put up (i.e. in the ON position)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

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.

1		<p>Check whether all DIP switches are put down (i.e. in the OFF position). If not, position them so now.</p>
2		<p>If OPUS is already installed...:</p> <ol style="list-style-type: none"> 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. <p>If OPUS is not yet installed...:</p> <ol style="list-style-type: none"> 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.
3		<ul style="list-style-type: none"> • Activate the <i>Search for instrument in network</i> option button. • Click the <i>Next</i> button.
4	<p>• Select the spectrometer from the list box.</p>  <p>i The list box contains all spectrometers connected to the network, or directly to a PC.</p> <ul style="list-style-type: none"> • 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. 	

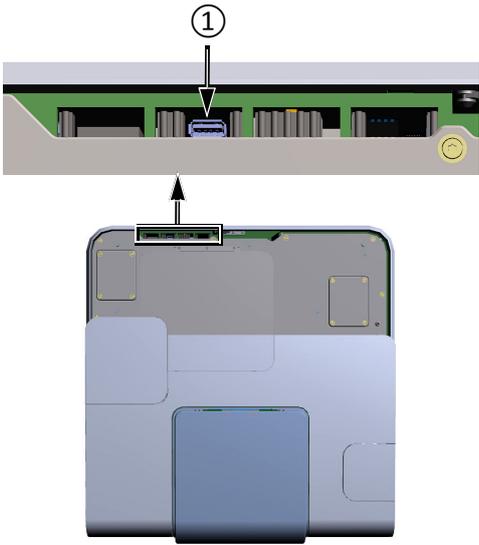
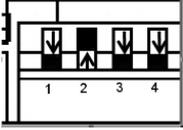
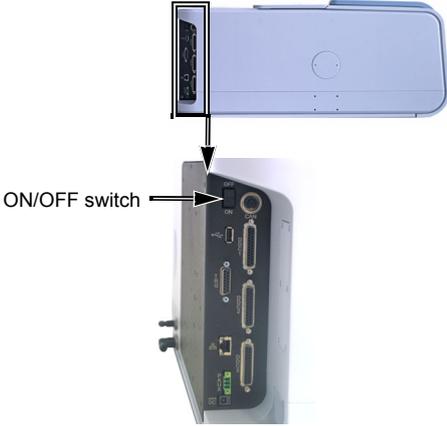
<p>5</p>	 <p>The screenshot shows the 'FCONF Firmware configuration tool' window. On the left, under 'Tasks', the 'Configure IP Settings' button is highlighted with a mouse cursor. On the right, under 'Devices', a table lists IP addresses and MAC addresses. The first row is selected:</p> <table border="1"> <thead> <tr> <th>IP Address</th> <th>MAC</th> </tr> </thead> <tbody> <tr> <td>149.236.31.1</td> <td>00:0</td> </tr> <tr> <td>149.236.31.1...</td> <td>00:0</td> </tr> <tr> <td>149.236.31.1</td> <td>00:0</td> </tr> </tbody> </table>	IP Address	MAC	149.236.31.1	00:0	149.236.31.1...	00:0	149.236.31.1	00:0	<p>Click the <i>Configure IP Settings</i> button.</p>
IP Address	MAC									
149.236.31.1	00:0									
149.236.31.1...	00:0									
149.236.31.1	00:0									
<p>6</p>	<ul style="list-style-type: none"> • Enter the IP address, subnet mask and gateway.  <p>The screenshot shows the 'Set IP Address' dialog box. It contains the following information:</p> <ul style="list-style-type: none"> IP settings controlled via DIP - switches on the instrument backpanel current IP settings: IP Address: 149 . 236 . 31 . 147, Subnet Mask: 255 . 255 . 255 . 0, Default Gateway: 149 . 236 . 31 . 1 Product: INVENIO-R, MAC Address: 00:00:ad:10:90:15 <p>An arrow points to the 'Apply' button.</p>	<ul style="list-style-type: none"> • Click the <i>Apply</i> button. 								
<p>7</p>	 <p>The screenshot shows the 'FCONF Firmware configuration tool' window. On the left, under 'Tasks', the 'Reboot Device' button is highlighted with a mouse cursor. On the right, under 'Devices', a table lists IP addresses:</p> <table border="1"> <thead> <tr> <th>IP Address</th> </tr> </thead> <tbody> <tr> <td>149.236.31.1</td> </tr> <tr> <td>149.236.31.1...</td> </tr> <tr> <td>149.236.31.1...</td> </tr> <tr> <td>149.236.138....</td> </tr> <tr> <td>149.236.138....</td> </tr> <tr> <td>149.236.31.1...</td> </tr> </tbody> </table>	IP Address	149.236.31.1	149.236.31.1...	149.236.31.1...	149.236.138....	149.236.138....	149.236.31.1...	<p>Click the <i>Reboot Device</i> button.</p>	
IP Address										
149.236.31.1										
149.236.31.1...										
149.236.31.1...										
149.236.138....										
149.236.138....										
149.236.31.1...										
<p>8</p>	 <p>The screenshot shows the 'Reboot Device' dialog box. It contains the following information:</p> <ul style="list-style-type: none"> Product Name: INVENIO-R MAC Address: 00:00:ad:0b:5d:15 Password: * To reboot your instrument, please press the reboot-button. 	<ul style="list-style-type: none"> • Click the <i>Reboot</i> button. • Click the <i>Close</i> button. ➤ The spectrometer reboots. After 30 to 60 seconds the list box, which contains all spectrometers connected to the network, is displayed again. 								

<p>9</p>		<p>Click the <i>Refresh List</i> button to refresh and check the entries in the list box.</p>
<p>10</p>		<ul style="list-style-type: none"> • Select the spectrometer IP address in the list box. • Click the <i>Select</i> button.
<p>11</p>	<p>The <i>IP address</i> field must now contain the updated IP address.</p> 	

3.8.6.4 Reassigning the standard IP address to the spectrometer

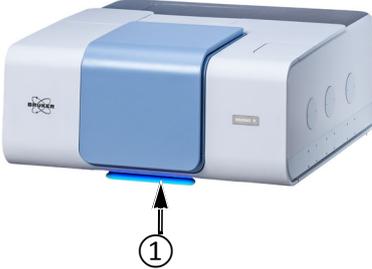
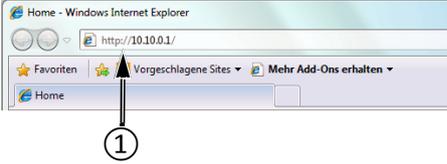
By default, the spectrometer is delivered with the factory-assigned standard IP address 10.10.0.1. This is the spectrometer IP address for the connection variants A and C, you do not need to assign a different IP address to the spectrometer.

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		<p>① - Location of the DIP switch</p> <p>☞ For information about how to get access to the DIP switch, see section 3.8.6.1.</p>
2		<p>Position the DIP switches as follows:</p> <ul style="list-style-type: none"> • 2nd DIP switch: up (ON status) • 1st, 3rd and 4th DIP switch: down (OFF status)
3		<p>Restart the spectrometer by switching it off and on again.</p>
4	<p>➤ After the spectrometer reboot is finished, the standard IP address (10.10.0.1) is assigned to the spectrometer.</p>	

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:

1		<p>Switch on the spectrometer using the ON/OFF switch ① at the spectrometer rear side.</p> <p>Switch on the PC.</p>
2		<p>Wait until the spectrometer and the PC have finished booting up and are ready to operate.</p> <p>Note: The status LEDs ① light up bluish only for the duration initialization of the spectrometer.</p> <p>➤ For detailed information about the status LEDs, see section 4.1.1.</p>
3	<p>Start an Internet browser.</p> <p>Check whether the Internet browser is not in the offline mode.</p> <p>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.</p>	
4		<p>Enter the spectrometer IP address in the Internet browser entry field ① and press the ENTER key.</p> <ul style="list-style-type: none"> • 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-r-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.

<p>5</p>	<p>INVENIO-R SN_28 Home</p> <ul style="list-style-type: none"> • Measurement Menus • Measurement Status • Direct Command Entry • Messages • Diagnostics • Service • Edit Owner/Company Data • Authentication <p>Page generated on Wed, 18 Apr 2018 11:33:53</p>	<p>☞ In case of a successful communication between spectrometer and PC, the Internet Explorer now displays the home page of your spectrometer firmware.</p>
	<p>☞ 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.</p>	

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

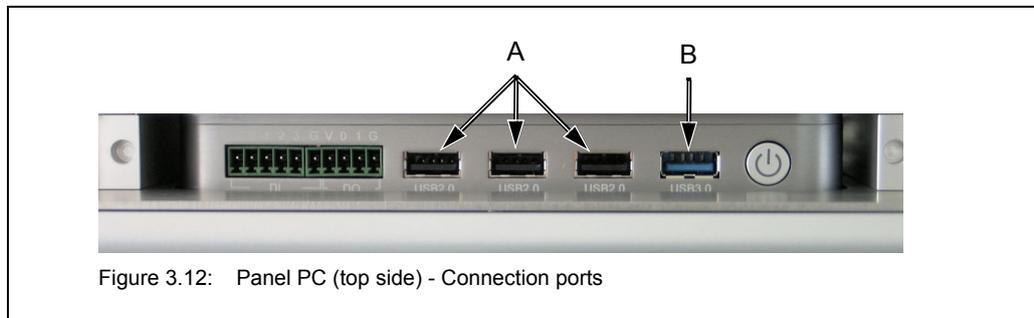


Figure 3.12: Panel PC (top side) - Connection ports

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

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.



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 installation 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 account¹ 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 password² 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

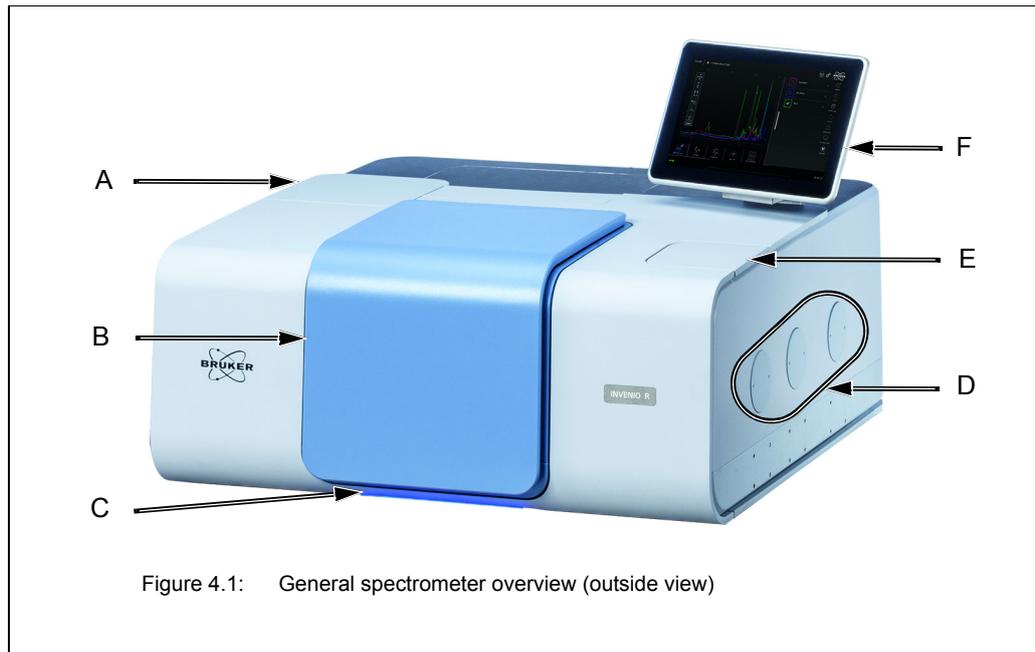
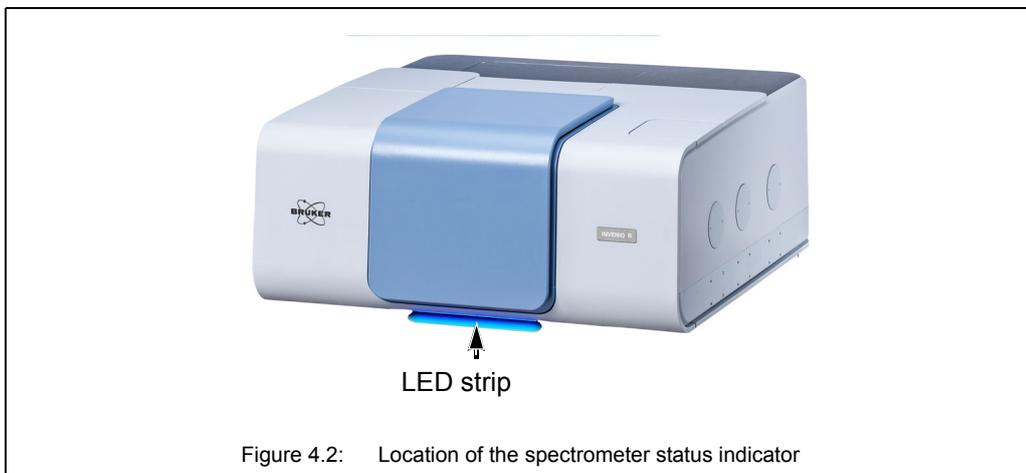


Fig. 4.1	Description
A	Cover providing access to the DigiTect-type detector
B	Cover providing access to the large-sized sample compartment
C	Spectrometer status indicator (LED strip below the sample compartment)
D	IR beam inlet and outlet ports
E	Cover providing access to the small-sized sample compartment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

4.1.1 Spectrometer status indicator



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.	<p>The spectrometer is initializing.</p> <p>Note: The LEDs light up bluish only for the duration of spectrometer initialization.</p>
LEDs light up blue.	<p>Instrument is OK and ready for measurement. This is the case when:</p> <ul style="list-style-type: none"> • 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.	<p>A yellow instrument status indicates a warning. This is the case when:</p> <ul style="list-style-type: none"> • 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. <p>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.</p> <p>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.</p>

<p>LEDs light up red.</p>	<p>A red instrument status LED indicates an error. For example, this is the case when:</p> <ul style="list-style-type: none"> • an optical component (e.g. NIR source, laser) fails or does not achieve its performance specification <p>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.</p> <p>☞ For a systematic fault diagnosis see section 7.3.</p>
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4.1.2 Sample compartments

The following sample compartments are available:

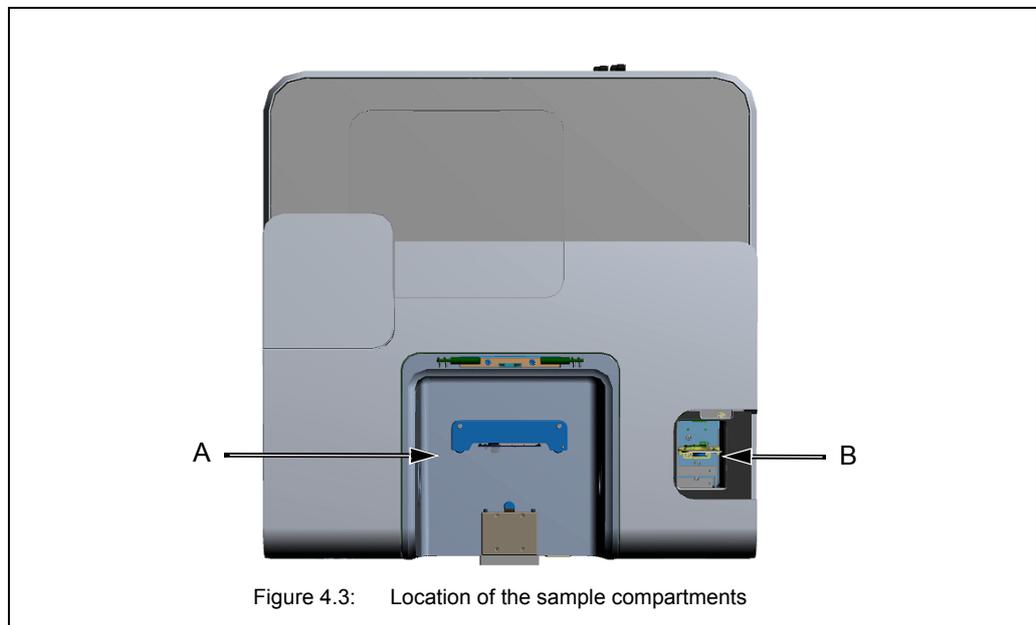
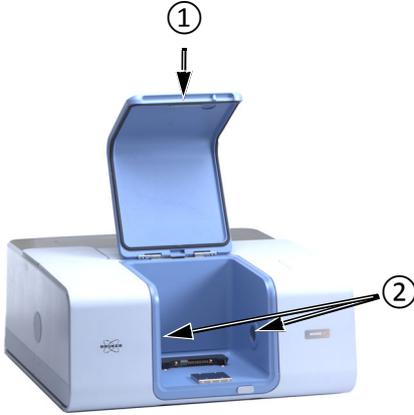
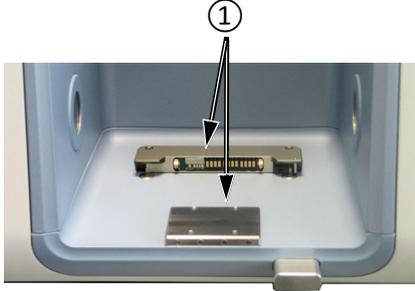


Figure 4.3: Location of the sample compartments

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

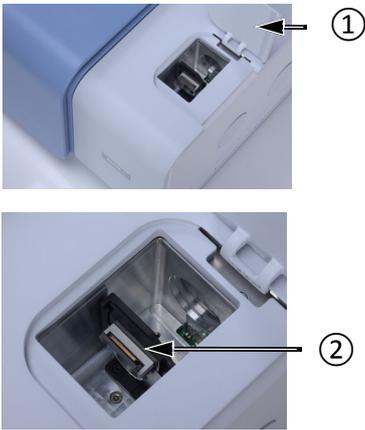
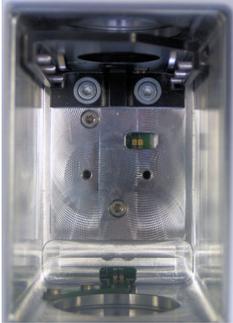
4.1.2.1 Sample compartment with QuickLock

	<p>Open the sample compartment by turning the sample compartment cover ① upwards.</p> <p>The circular openings ② on either side of the sample compartment are closed either by windows or automatic shutters.</p> <ul style="list-style-type: none"> ☞ For information about the available window materials, see section 4.5.5. ☞ For information about how to exchange a window, see section 5.12. ☞ For information about the automatic shutters, see section 5.4.5 and section 5.8.
	<p>To install bulky accessories inside the sample compartment you can remove the sample compartment cover by pressing the release button ...</p> <p>...while taking off the cover.</p>
	<p>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.</p> <ul style="list-style-type: none"> ☞ 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.

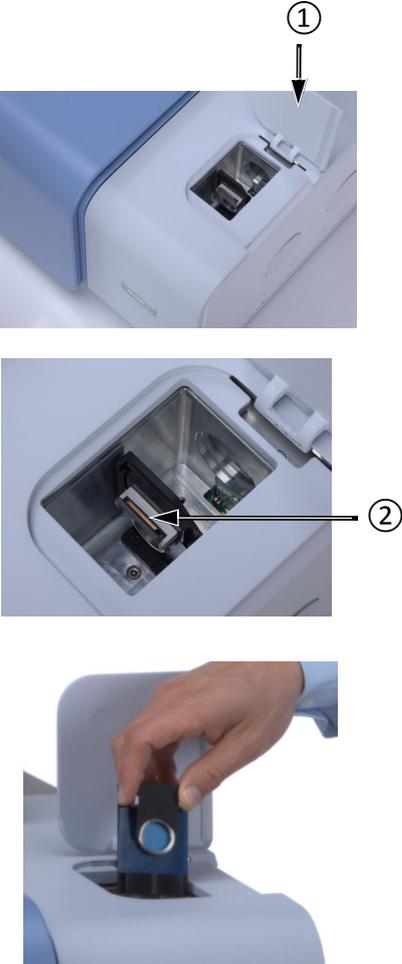
	<p>Open the sample compartment by turning the sample compartment cover ① upwards.</p> <p>This sample compartment is equipped with a slide bracket ② to slide in the available accessories.</p>
	<p>A variety of sample accessories is available: Pellet holder, magnetic holder for films, clamp holders for different kind of flat samples, gas and liquid cells etc.</p>
<p>Depending on the accessory to be used, the slide bracket can be relocated between the following two positions:</p>	
	<p>Slide bracket in the rear position when using the following accessories: gas cell and reflection unit</p>
	<p>Slide bracket in the center position when using the following accessories: pellet holder, foil holder and liquid cell</p>
<p>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.</p>	

The following figure illustrates how to use the available accessories.



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.

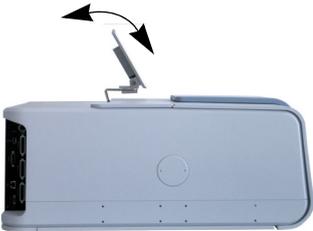
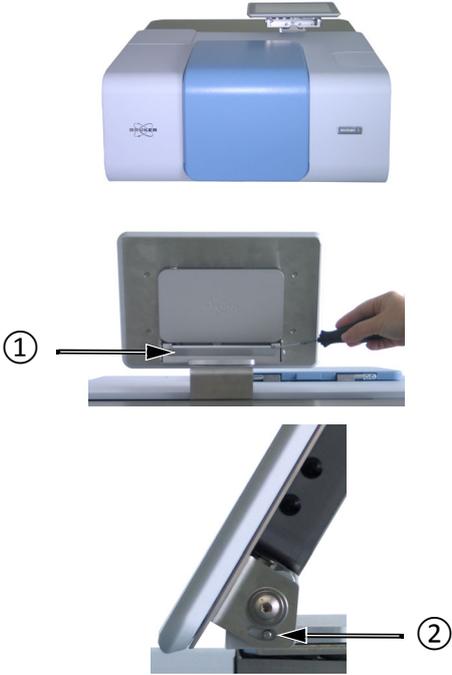
 <p>The diagram consists of three vertically stacked images. The top image shows a hand lifting the white sample compartment cover, indicated by a circled '1' and a downward arrow. The middle image shows the interior of the compartment with a black sample holder, indicated by a circled '2' and an arrow. The bottom image shows a hand inserting a blue sample holder into the compartment.</p>	<p>Open the sample compartment by turning the sample compartment cover ① upwards.</p> <p>This sample compartment is equipped with a sample holder ② for transmission measurements only. The sample holder is fixedly mounted in the sample compartment i.e. it cannot be exchanged for other measurement accessories.</p> <p>Pellet holders, magnetic holders for films, clamp holders for different kind of flat samples and liquid cells can be used.</p>
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4.2 Panel PC with touch screen

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

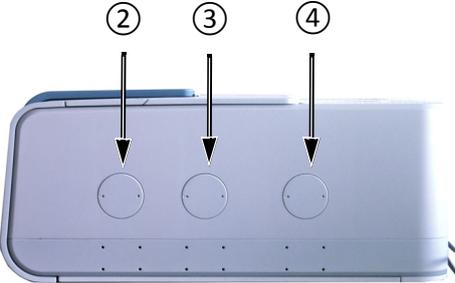
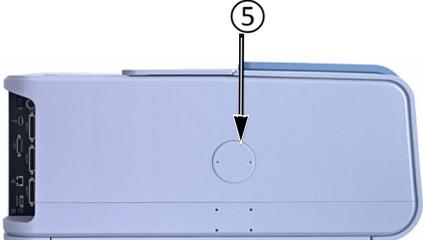
For detailed information about the OPUS/TOUCH software, refer to the OPUS/TOUCH Manual.

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

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

4.3 IR beam ports

The spectrometer has five IR beam ports - three IR beam outlet ports and two IR beam inlet ports - allowing the coupling / connection of accessories and/or components (e.g. FT-IR microscope, Raman module, light source) to the spectrometer. (See section 2.6.)

 <p>①</p>	<p>Spectrometer rear side</p> <p>① - Inlet port for connecting a light emission source (e.g. Hg source)</p>
 <p>② ③ ④</p>	<p>Right spectrometer side</p> <p>② - Outlet port for a parallel IR-beam (Note: This port cannot be used if the spectrometer has an optional, small-sized sample compartment.)</p> <p>③ - Outlet port for a parallel IR-beam (e.g. for connecting the FT-IR microscope HYPERION, PMA50 or external sample compartment XSA)</p> <p>④ - Inlet port for connecting a light emission source (e.g. FT Raman module RAM II or a water-cooled, high-power MIR source)</p>
 <p>⑤</p>	<p>Left spectrometer side</p> <p>⑤ - Outlet port for a parallel IR-beam (e.g. for connecting the FT-IR microscope HYPERION or an external detector chamber)</p>

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

	<p>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.3.) 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.</p>
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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

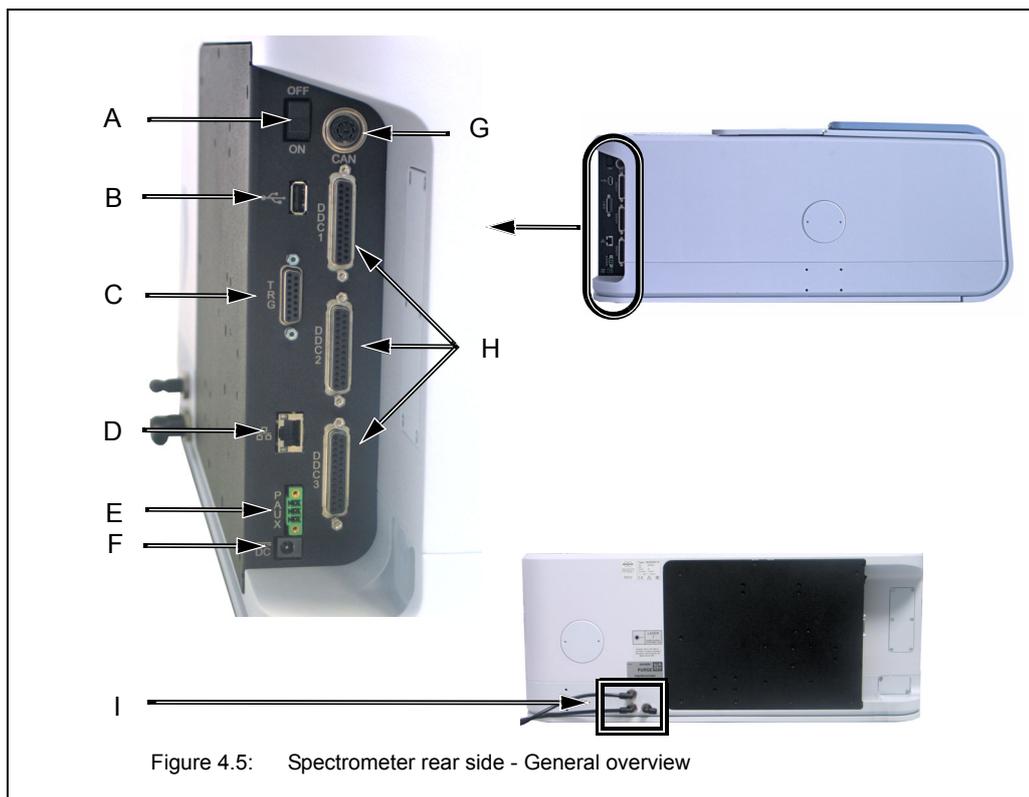


Figure 4.5: Spectrometer rear side - General overview

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	<p>Ethernet port</p> <p>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.</p> <p>☞ For detailed information, see section 3.8.</p>
E	<p>PAUX port for power supply of externally connected accessories</p>
F	<p>Low-voltage socket</p> <p>The low-voltage socket is used to connect the low-voltage cable of the external power supply unit to spectrometer.</p> <p>☞ For information about how to connect the spectrometer to the mains power supply, see section 3.6.</p>
G	<p>CAN bus port (for connecting motorized accessories)</p> <p>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.)</p>
H	<p>DDC1 to DDC3 ports</p> <p>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.</p>
I	<p>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)</p> <p>☞ Note: For information about how to connect the spectrometer to a purge gas supply line, see section 3.7.</p>

4.5 Inside view

4.5.1 Overview

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

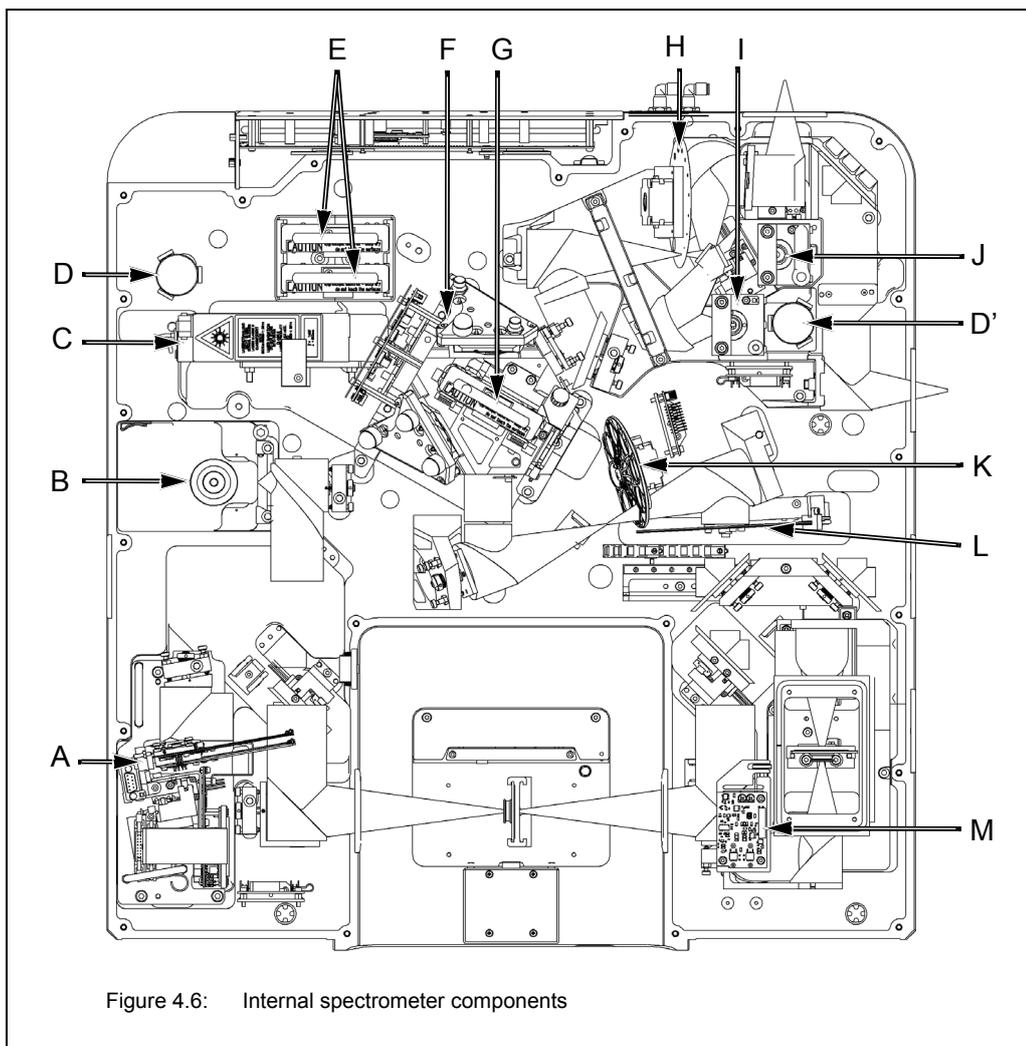


Figure 4.6: Internal spectrometer components

Fig. 4.6	Internal spectrometer component
A	<p>Multi-detector unit</p> <p>Standard: Multi-detector unit with one room temperature DTGS</p> <p>Option: Multi-detector unit with several room temperature detectors</p> <p>Note: The multi-detector unit can be equipped with up to five room temperature detectors.</p>
B	<p>Detector (DigiTect-type)</p> <p>Note: At this position, either a MCT or DLaTGS detector can be installed.</p>

Fig. 4.6	Internal spectrometer component
C	Laser
D & D'	Desiccant cartridges
E	2x Beamsplitters (in storage position)
F	RockSolid interferometer block
G	Beamsplitter (in operation position)
H	Aperture wheel
I	NIR source
J	MIR source
K	Filter wheel (IVU - <u>I</u> nternal <u>V</u> alidation <u>U</u> nit) 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.
L	Attenuator wheel (It is a perforated grid wheel with different sieve sizes / grid sizes for an additional attenuation of the IR beam.) The attenuator wheel is an optional feature.
M	Detector unit of the small-sized sample compartment (room temperature DTGS)

4.5.2 Source

Standard source

The basic spectrometer configuration is equipped by default with a MIR source which is installed inside the spectrometer (J in fig. 4.6). The MIR source is a globar (i.e. an U-shaped silicon carbide piece) that 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.

The advanced spectrometer configuration is equipped by default with a MIR source (J in fig. 4.6) and a NIR source (I in fig. 4.6). Both sources are installed inside the spectrometer. The selection of source to be used is realized by using OPUS. (See appendix C.)

Optional sources

The available optional sources provide for different spectral ranges. Note that the combination of source, detector and beamsplitter defines the IR measurement range.

Type of source	Mode of cooling	Installation location
VIS/NIR source (tungsten halogen lamp)	air-cooled	installed in the spectrometer (I in fig. 4.6)
FIR source (mercury lamp)	water-cooled ^a	connected externally to the spectrometer
UV/VIS/NIR source (tungsten lamp)	water-cooled ^a	connected externally to the spectrometer
High-power MIR source (globar)	water-cooled ^a	connected externally to the spectrometer

a. For the usage of a water-cooled source, a cooling device with closed water circulation is included in the delivery scope.

All external sources can be connected to either of the two IR beam inlet ports (A or B in fig. 4.7).

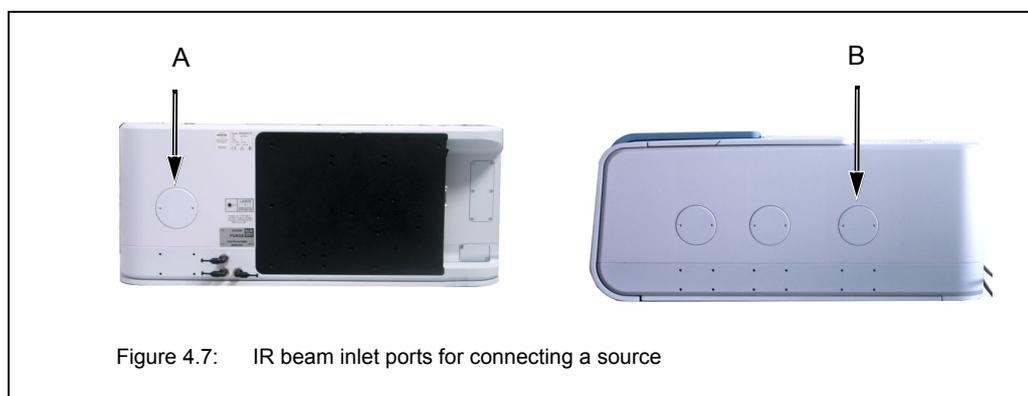


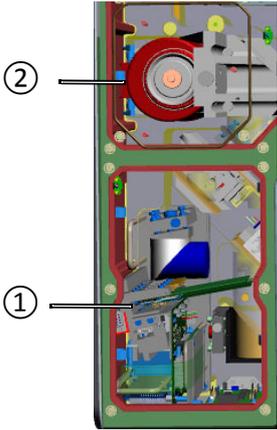
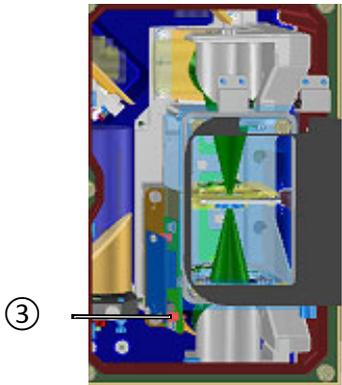
Figure 4.7: IR beam inlet ports for connecting a source

If the spectrometer is equipped with several sources, select in OPUS the source which is to be used for the measurement. (See appendix C.)

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.

	<p>The spectrometer can be equipped with the following detectors:</p> <ul style="list-style-type: none"> ① - Multi-detector unit (Standard: The unit is equipped with one room temperature DTGS detector. Option: The unit can be equipped with up to five Multi-Tect-type detectors.) 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 5.11. <p>➤ These detectors are available for measurements performed with the large-sized sample compartment.</p>
	<p>For measurements performed with the small-sized sample compartment, the following detector is available:</p> <ul style="list-style-type: none"> ③ - DTGS detector (room temperature)
	<p>At the IR beam outlet port ④ at the left spectrometer side, an optional bolometer detector can be connected.</p>
<p>The detector which is used for the measurement is selected by the user in OPUS.</p>	

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

The spectrometer is equipped with a multi-detector unit which can include up to five detectors. For the multi-detector unit, the following MultiTect-type detectors are available:

Detector	Spectral range (cm ⁻¹)	Sensitivity	Operating temperature / cooling method
Mid-Infrared			
DLaTGS with KBr window	12,000 - 350	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	room temperature (Note: Temperature stabilization is an optional feature.)
DLaTGS with CsI window	12,000 - 130	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Room temperature, no cooling required
Near-Infrared			
InGaAs diode	12,800 - 4,000	NEP: $< 5 \times 10^{-12} \text{ W Hz}^{-1/2}$	Room temperature, no cooling required
InGaAs diode	12,800 - 4,000	NEP: $< 2 \times 10^{-13} \text{ W Hz}^{-1/2}$	Peltier-cooled
Far-Infrared			
DLaTGS with PE window	700 - 10	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Room temperature, no cooling required
Far- and Mid-Infrared			
Wide range DLATGS	12,000 - 20	No NEP available	Room temperature, no cooling required
Visible & UV			
Silicon diode	25,000 - 9,000	NEP: $< 10^{-14} \text{ W Hz}^{-1/2}$	Room temperature, no cooling required
GaP diode	28,000 - 18,000	No NEP available	Room temperature, no 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	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	room temperature (Note: Temperature stabilization is an optional feature.)

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

For installing a DigiTect-type detector, there is an additional detector position which is an optional feature. The optionally available DigiTect-type detectors provide for different spectral ranges and sensitivities. Note that the combination of source, detector and beamsplitter defines the IR measurement range.

The following DigiTect detectors are available:

Detector	Spectral range (cm ⁻¹)	Sensitivity	Operating temperature / cooling method
Mid-Infrared			
DLaTGS with KBr window	12,000 - 350	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	temperature stabilized
DLaTGS with CsI window	12,000 - 130	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Room temperature
MCT narrow band, with BaF ₂ window HARMFUL!	12,000 - 850	$D^* > 4 \times 10^{10} \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
MCT mid band, with ZnSe window TOXIC!	12,000 - 600	$D^* > 2 \times 10^{10} \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
MCT broad band, with KRS-5 window TOXIC!	12,000 - 420	$D^* > 5 \times 10^9 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
Photovoltaic MCT, with BaF ₂ window HARMFUL!	12,000 - 850	$D^* > 3 \times 10^{10} \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
MCT/InSb Sandwich, with ZnSe window TOXIC!	10,000 - 600	$D^* > 2 \times 10^{10} \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
Near-Infrared			
InSb	10,000 - 1,850	$D^* > 1.5 \times 10^{11} \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
InSb with cold filter	10,000 - 3,500	$D^* > 5 \times 10^{11} \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Liquid N ₂ cooled
Ge detector (Raman)	11,750 - 5,900	NEP: $< 10^{-15} \text{ W Hz}^{-1/2}$	Liquid N ₂ cooled
InGaAs diode	12,800 - 5,800	NEP: $< 2 \times 10^{-14} \text{ W Hz}^{-1/2}$	Room temperature
InGaAs diode	12,800 - 4,000	NEP: $< 2 \times 10^{-13} \text{ W Hz}^{-1/2}$	Peltier cooled
Far Infrared			
DLaTGS with PE window	700 - 10	$D^* > 4 \times 10^8 \text{ cm Hz}^{1/2} \text{ W}^{-1}$	Room temperature
Silicon bolometer ^a	600 - 10	NEP: $< 10^{-13} \text{ W Hz}^{-1/2}$	Liquid He cooled
Far- and Mid-Infrared			
Wide range DLATGS	12,000 - 20	No NEP available	Room temperature

Detector	Spectral range (cm ⁻¹)	Sensitivity	Operating temperature / cooling method
Visible & UV			
Silicon diode	25,000 - 9,000	NEP:<10 ⁻¹⁴ W Hz ^{-1/2}	Room temperature
GaP diode	28,000-18,000	No NEP available	Room temperature

a. The silicon bolometer is connected externally to the outlet port at the left spectrometer side.

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 5.11.

4.5.4 Beamsplitter

Standard beamsplitter

The basic spectrometer configuration is equipped with a KBr beamsplitter which covers a spectral range from 8,000 to 350 cm^{-1} .

Optional beamsplitters

The available optional beamsplitters provide for different spectral ranges. Note that the combination of source, detector and beamsplitter defines the IR measurement range. The following optional beamsplitters are available:

Beamsplitter	Spectral range (cm^{-1})	Color coding of the beamsplitter handle
Mid-infrared		
KBr (standard)	8,000 - 350	red
KBr (broad band)	10,000 - 380	red
Near-infrared		
CaF ₂ HARMFUL!	15,000 - 1,200	black
Visible & UV		
Quartz VIS/UV	30,000 - 3,500	white
Far-infrared		
Multilayer (far IR)	680 - 30	metallic
Mylar 25 μm	120 - 30	metallic
Mylar 50 μm	55 - 10	metallic
Solid state beamsplitter based on silicon plate	600 - 30	metallic
Mid- and far-infrared		
Wide range beamsplitter	6,000 - 10	metallic
Alignment tool		
Glass	For alignment purposes only!	metallic

WARNING

Health hazard because of improper handling of broken harmful beamsplitter material

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

- > Avoid generating dust of broken beamsplitter material. The material is harmful if swallowed or inhaled.
- > Also avoid skin and eye contact.
- > Dispose the harmful 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.

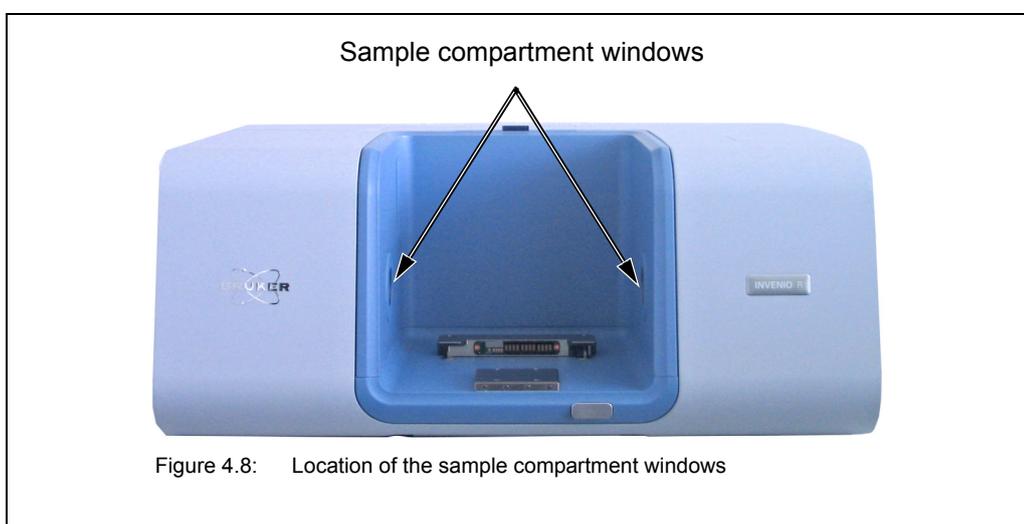


4.5.5 Sample compartment windows

General information

There is a circular opening on either side of the large-sized sample compartment. (See fig. 4.8.) 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, 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.



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 2000cm ⁻¹)	Chemical properties
Quartz (Infrasil), SiO ₂	57,000 - 2,800	1.46	Insoluble in water; soluble in HF
Calcium Fluoride, CaF ₂	66,000 - 1,000	1.40	Insoluble in water; resistant to most acids and bases; soluble in NH ₄ solutions
Barium Fluoride, BaF ₂ HARMFUL!	50,000 - 800	1.45	Low water solubility; soluble in acid and NH ₄ Cl solutions
Sodium Chloride, NaCl	28,000 - 580	1.50	Hygroscopic; slightly soluble in alcohol and NH ₃

Material	Transmission range (cm ⁻¹)*	Refraction index n (at 2000cm ⁻¹)	Chemical properties
Zinc Selenide, ZnSe TOXIC!	20,000 - 500	2.43	Soluble in strong acids and in HNO ₃
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
KRS-5 (TlBr/I thallium bromide-iodide) VERY TOXIC!	16,000 - 250	2.38	Soluble in warm water and bases; insoluble in acids
Polyethylene PE (high density)	600 - 10	1.52	Resistant to most solvents

50% value at a window thickness of 4mm

Some sample compartment windows are of a material which is harmful or (very) 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.

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 5.12.

4.5.6 Laser

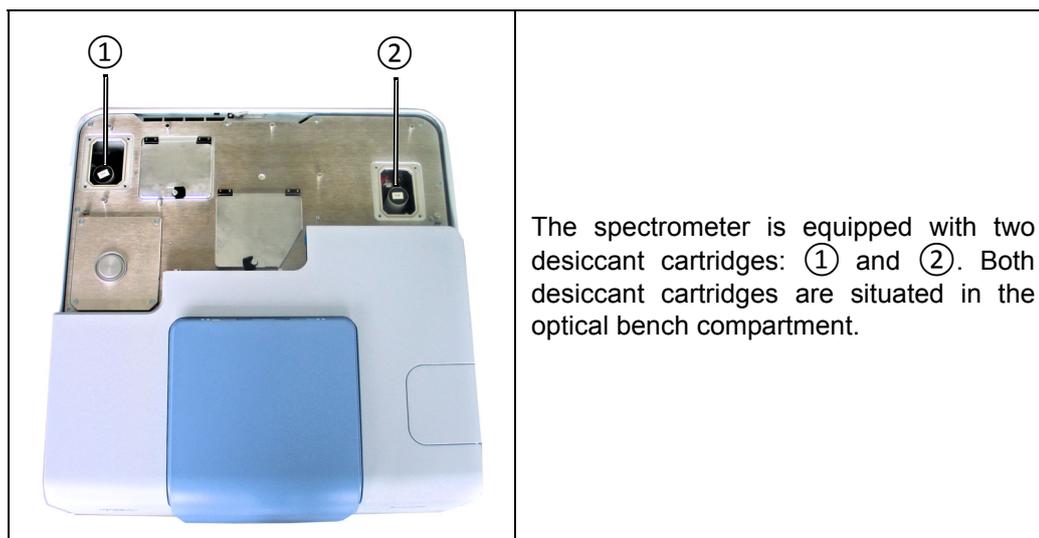
The spectrometer is equipped with a HeNe laser (C in fig. 4.6) that emits red light with a wavelength of 633 nm and has a rated power output of 0.8 mW.

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 HeNe 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 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, H₂O 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.

4.6 Optical beam path

The actual beam path is determined by:

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

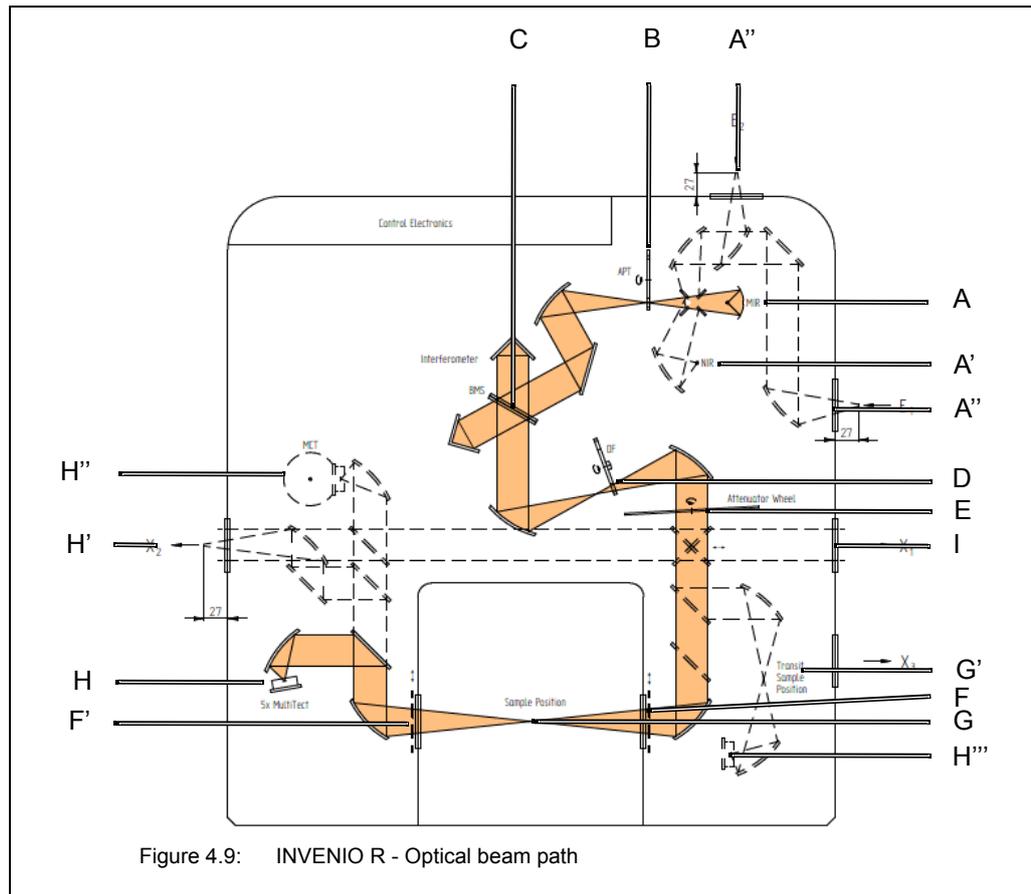


Fig. 4.9	Explanation
A	MIR source
A'	NIR source
A''	IR beam inlet for an externally installed source
B	Aperture wheel Note: The aperture wheel has 12 default wheel positions with aperture diameters ranging from 0.25 mm to 8 mm.
C	Interferometer block with integrated beamsplitter
D	Optical filter wheel (IVU - Internal Validation Unit), filter diameter: 25 mm

Fig. 4.9	Explanation
E	Attenuation wheel (optional component)
F	Sample compartment window (IR beam entrance into the large-sized sample compartment)
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	Detector (MultiTect-type), in case the large-sized sample compartment is used Standard: Multi-detector unit with one room temperature DTGS detector Option: Multi-detector unit with up to five detectors
H'	IR beam outlet for an externally installed detector (e.g. bolometer)
H''	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)

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
- exchanging the beamsplitter (for the purpose of changing the spectral range)
- installing / exchanging a DigiTect-type detector (for the purpose of changing the spectral range)
- exchanging the sample compartment window (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

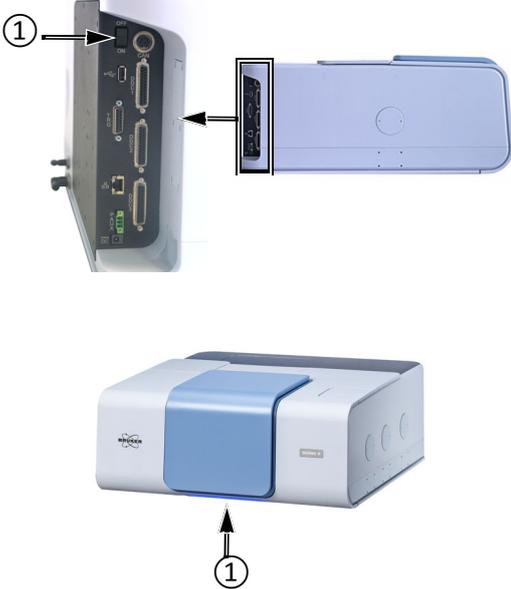
Specifying the measurement parameters and starting a measurement and evaluating the measurement results as well as defining and starting a spectrometer validation test (OQ and PQ) are done exclusively using the spectroscopic software program OPUS.

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

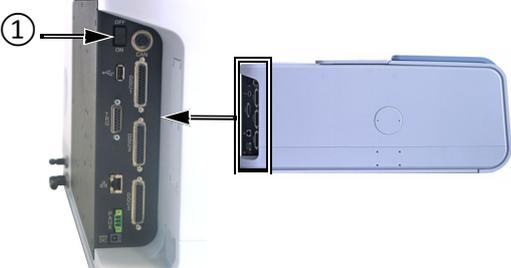
The standard spectrometer configuration is designed for measurements in the mid infrared region. Optionally, the spectral range can be expanded by exchanging the installed MIR components (detector and beamsplitter, sample compartment windows) for the corresponding optical components that allow measurements in the far or near infrared as well as in the visible or ultraviolet region.

☞ For information about the substitution procedure of these optional components refer to the corresponding sections in this chapter.

5.2 Switching on the spectrometer system

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

5.3 Switching off the spectrometer system

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

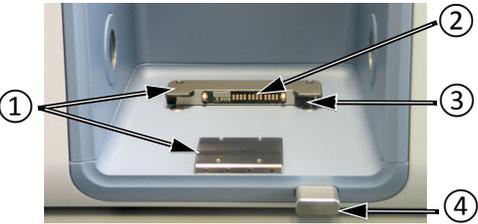
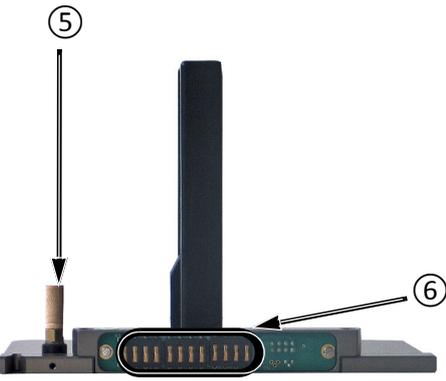
i Switch off the spectrometer only in case of a long time of non-use. We recommend keeping the spectrometer in the on-state overnight and over the weekend. Reason: After being switched on again, the spectrometer is ready for measurement after about 15 minutes. For high-precision measurements, however,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

	<p>Spectrometer sample compartment (inside view)</p> <ul style="list-style-type: none"> 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
	<p>Standard sample holder with QuickLock baseplate</p> <ul style="list-style-type: none"> ⑤ - Purge gas diffuser 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 ①) <p>Note: This sample holder for transmission measurements is included in the standard delivery scope of the spectrometer.</p>

5.4.2 Putting an accessory in the sample compartment

1		<p>Press the QuickLock button.</p> <p>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.</p> <p>While inserting the accessory in the QuickLock mechanism, tilt the accessory QuickLock baseplate front edge slightly upwards.</p>
2		<p>Press the QuickLock button for the accessory to lock in place.</p>
3	<p>➤ As soon as the accessory QuickLock baseplate locks in place, the electronic connections for AAR are established. This is indicated by a beep.</p>	

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 test¹ using OVP².

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	<ul style="list-style-type: none"> ☞ 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.	<ul style="list-style-type: none"> ☞ For information about how to insert a Quick-Lock-type accessory into the spectrometer sample compartment, see the section 5.4. <hr/> <p>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.</p> <hr/>
3	Equilibrate purge.	<p>Before starting the background measurement, make sure that the purge has sufficiently removed the water vapor from the IR-beam path.</p> <p>Depending on the geometry and the volume of the accessory optics, the equilibration will take several minutes after an accessory exchange.</p> <p>Note: In case the equilibration of the purge has been insufficient, the sample spectrum will contain water bands.</p> <ul style="list-style-type: none"> ☞ 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).	<p>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.</p> <hr/> <p>➤ In case you intend to measure the sample with an ATR accessory, perform the background measurement with an empty ATR crystal.</p> <p>➤ 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.</p> <p>🔍 For detailed information about sample preparation refer to appendix F.</p>
5	Put the sample in the sample compartment by positioning the sample in the measurement position.	
6	In OPUS, start a sample measurement.	<p>🔍 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.</p> <p>➤ Afterwards, OPUS calculates automatically the result sample spectrum by dividing the sample spectrum (acquired in step 7) by the background spectrum (acquired in step 4).</p> <p>🔍 For detailed information about the OPUS functions for data acquisition, manipulation and evaluation refer to the OPUS Reference Manual or OPUS/TOUCH Manual.</p>

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

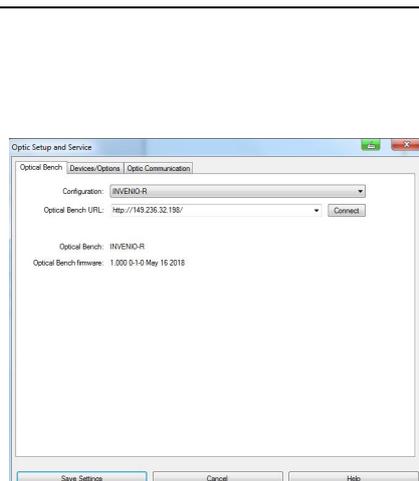
- **Important:** Both the integrated panel PC and the externally connected PC data station must use the same OPUS/IR version to avoid compatibility problems!

	<p>INVENIO with integrated panel PC (optional feature) connected to a PC data station</p> <p>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.</p>
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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

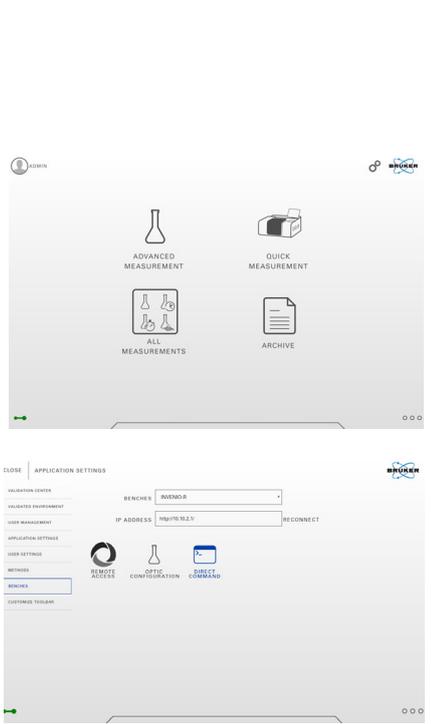
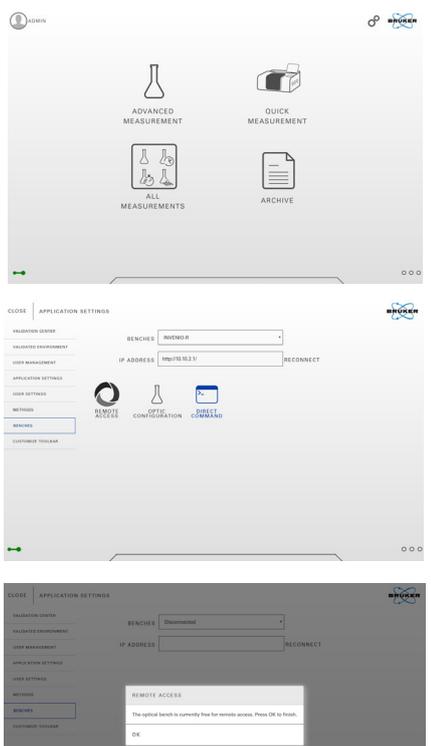


Connecting with the spectrometer

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-R.
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-r-SN* with *SN* being the serial number of the spectrometer in question (e.g. *invenio-r-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 *No optical bench connected*.

Integrated panel PC with OPUS/TOUCH software	
	<p>OPUS/TOUCH provides two variants for connecting with the spectrometer and disconnecting.</p> <p>1. Conventional variant:</p> <p>Connecting with the spectrometer</p> <ol style="list-style-type: none"> OPUS/TOUCH home screen: Tap the  icon. In the view that opens, tap BENCHES. Select the spectrometer and enter the spectrometer IP address. Tap RECONNECT. <ul style="list-style-type: none"> ➤ If the connection between spectrometer and panel PC has been established, the  icon is shown at the lower left edge of the home screen. <p>Disconnecting</p> <ol style="list-style-type: none"> Return to the OPUS/TOUCH home screen. OPUS/TOUCH home screen: Tap the  icon. In the view that opens, tap BENCHES. In the BENCHES drop-down list, select Disconnected.
	<p>2. Variant: Disconnecting and reconnecting via Remote Access</p> <p>Disconnecting</p> <ol style="list-style-type: none"> OPUS/TOUCH home screen: Tap the  icon. In the view that opens, tap BENCHES. Tap the  icon. <ul style="list-style-type: none"> ➤ Now the connection between the panel PC and the spectrometer is interrupted and the PC data station can connect with the spectrometer. <p>Reconnecting</p> <ol style="list-style-type: none"> 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. <ul style="list-style-type: none"> ➤ 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 interferences 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, H₂O 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 H₂O and CO₂ 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 H₂O and CO₂ 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 H₂O and CO₂ inside the spectrometer is important but a constant concentration of these gases during both the background and the sample measurement, i.e. the H₂O and CO₂ 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 H₂O and CO₂ 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 (purge 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 Changing the spectral range

5.9.1 General information

The spectral range in which the spectrometer is capable of detecting an IR signal is determined by the following optical spectrometer components:

- source,
- beamsplitter,
- sample compartment windows and
- detector.

Consequently, changing the spectral range involves the exchange of some of these components. For information about how to substitute these optical components refer to the section 5.10 for exchanging the beamsplitter, section 5.11 for exchanging the Digi-Tect-type detector and section 5.12 for exchanging the windows.

- ☞ Bruker provides preconfigured spectral range packages which include the corresponding optical components. For information about the available preconfigured spectral range packages, see section 2.2.
- After having replaced one or more of the above listed optical components, it is highly recommended to validate the spectrometer performance by performing a PQ test using OVP. (See OPUS Reference Manual.)

The spectral ranges of the available sources, beamsplitters, detectors and sample compartment windows are listed in section 4.5.2 (source), section 4.5.3 (detector), section 4.5.4 (beamsplitter) and section 4.5.5 (sample compartment window).

- ☞ **Important: Make sure that the spectral ranges of the installed optical components correspond with each other!**

5.9.2 Automatic component recognition (ACR)

The optical spectrometer components source, beamsplitter, detector and sample compartment window are electronically coded enabling the spectrometer firmware to recognize automatically the type of source, beamsplitter and detector that is actually installed. The information about the installed optical components is passed on to the spectroscopy software OPUS. This feature is called ACR (Automatic Component Recognition). Its purpose is to prevent you from selecting a wrong component in OPUS when you set up a measurement experiment. (Note: A wrongly selected component is indicated in OPUS by a red colored entry field of the corresponding drop-down list. See also the OPUS Reference Manual.)

5.10 Exchanging the beamsplitter

☞ All available beamsplitters are listed in section 4.5.4.

5.10.1 Handling instructions

NOTE

Irreversibly damaged beamsplitter because of improper handling

The beamsplitter is a very delicate component. Observe the following handling instructions to ensure a long service life.

- Do not touch the optical material of the beamsplitter as this can damage it irreversibly. Take hold of the beamsplitter only by the handle. (See fig. 5.1).
- The optical material of some beamsplitters are hygroscopic. Do NOT expose them to humidity or water vapor. Store the beamsplitter under dry conditions, for example in a sealed container or in a dry environment (e.g. in the storage position inside the spectrometer, see E in fig. 4.6).
- Do not try to clean the optical material of the beamsplitter as this will definitively damage the beamsplitter irreversibly.
- Do not expose the beamsplitter (especially KBr beamsplitters) to temperature changes.
- Handle the beamsplitter with care. Avoid any kind of mechanical impact like stroke or falling down.
- Do not try to loosen or fasten the screws as this will impair the optical quality of the beamsplitter.

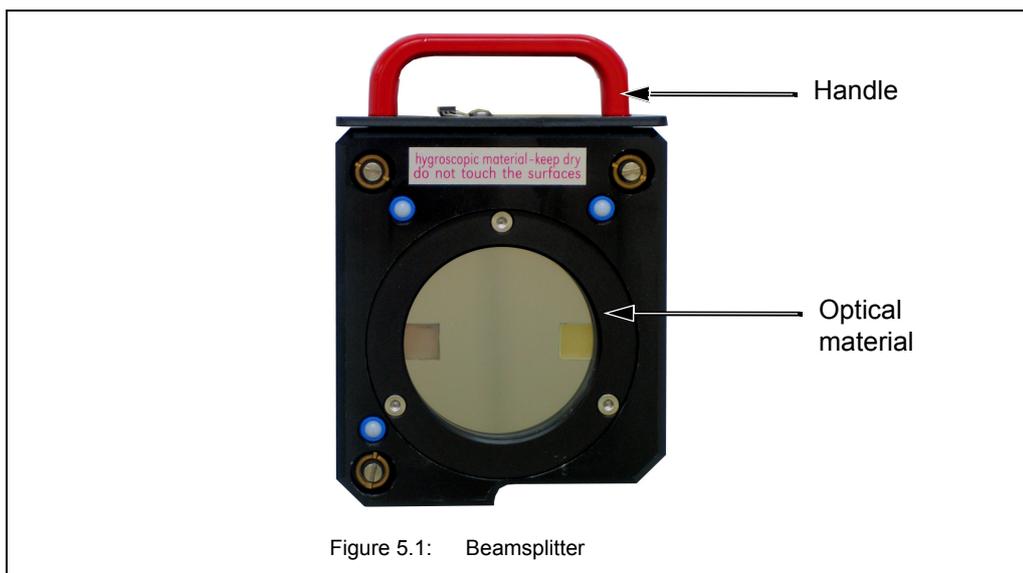
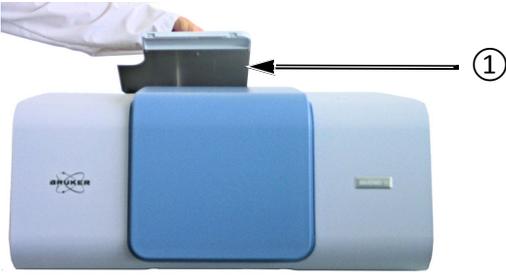
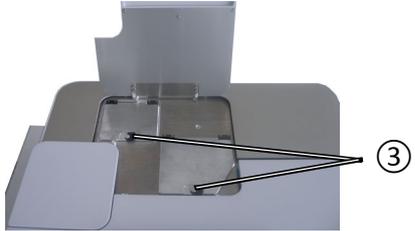
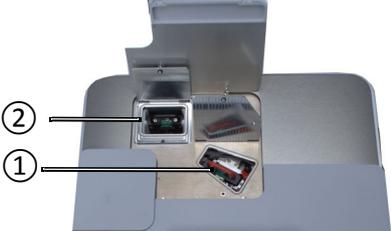
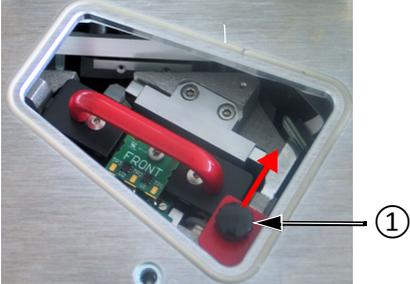
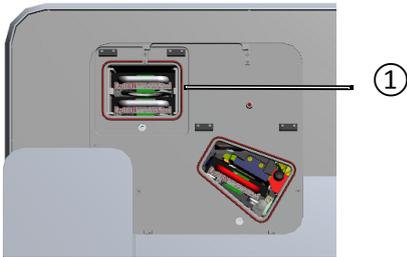
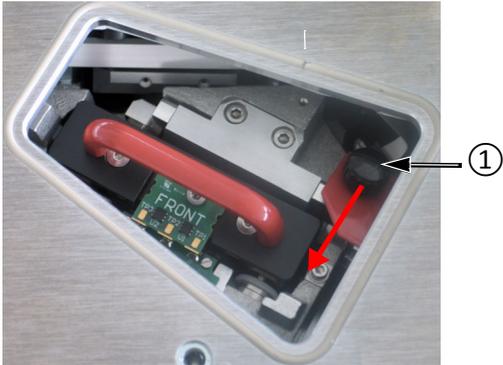
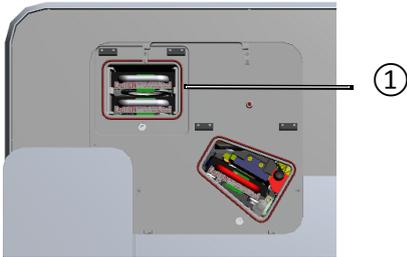
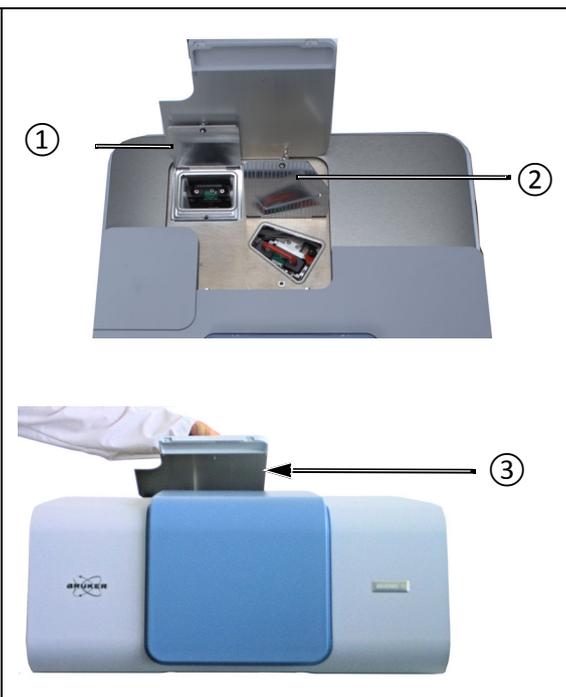
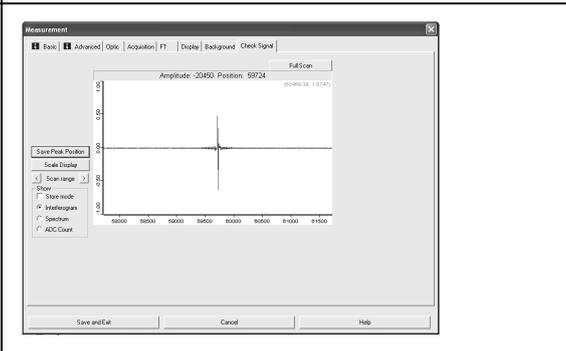


Figure 5.1: Beamsplitter

5.10.2 Exchange procedure

1	  	<p>To gain access to the beamsplitter:</p> <ol style="list-style-type: none"> 1. Fold back the outer lid ①. 2. Open the inner lids which provide access to the beamsplitter in the operating position ① and to the beamsplitter in the storage position ②, provided that the beamsplitter you intend to use is stored there. To do this, turn the spring-loaded quarter-turn fasteners ③ counterclockwise and open the lids.
2	 	<p>To remove the beamsplitter:</p> <ol style="list-style-type: none"> 1. Unlock the beamsplitter by moving the lever ① into the unlocked position (i.e. backwards). 2. Take the beamsplitter straight upwards out of the holder (operating position) without catching an edge.

3		<p>➤ Note: The exchange beamsplitter is stored either inside the spectrometer in the storage position ① or in a separate airtight storage box (outside the spectrometer).</p> <p>In the first case, take the beamsplitter out of the storage position holder.</p>
4	 	<p>To install the beamsplitter</p> <ol style="list-style-type: none"> 1. Insert the beamsplitter in the operating position holder with the electrical contacts facing to the spectrometer front side. Push down the beamsplitter completely until you feel resistance. <p>Attention! Insert the beamsplitter carefully in the holder. Do not drop the beamsplitter in the holder. Hitting too hard on the ground will damage the beamsplitter!</p> <ol style="list-style-type: none"> 2. Lock the beamsplitter by moving the lever ① into the locked position (i.e. forwards). <ul style="list-style-type: none"> ➤ A precise locking mechanism fixes the beamsplitter automatically at exact operating position. ➤ A beep indicates that the beamsplitter has been recognized by the electronics. ➤ After a few seconds the spectrometer starts to scan.
5		<p>Store the removed beamsplitter under dry conditions: Either insert the beamsplitter into the storage position holder ① inside the spectrometer or put it in the storage box which is intended for storing the beamsplitter outside the spectrometer.</p>

<p>6</p>		<p>Close the spectrometer:</p> <p>Close the inner lids ① and ② and turn the spring-loaded quarter-turn fasteners clockwise.</p> <p>Important note: While the inner lids are open, humid ambient air enters the optical bench. Therefore, always close these two lids immediately after having exchanged the beamsplitter. Make sure that the lids are closed properly!</p> <p>Fold down the outer lid ③.</p>
<p>7</p>		<p>Check the signal: Open the OPUS software program and check whether a signal is detected and whether the signal intensity is OK. (See section 5.13.)</p>

5.11 Exchanging a DigiTect-type detector

5.11.1 General information

Only the **advanced spectrometer** configuration has a dovetail-type detector position which allows for exchanging DigiTect-type detectors (e.g. MCT).

In case your measurement requires a different spectral range or another detection sensitivity than the installed MultiTect-type detectors allow, you can install in addition a DigiTect-type detector having the desired detection sensitivity and/or covering the desired spectral range.

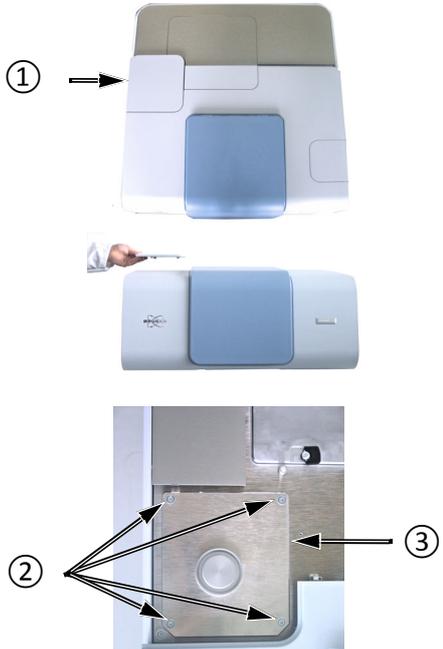
☞ In section 4.5.3, all available detectors are listed including their detection sensitivity and the spectral range they cover.

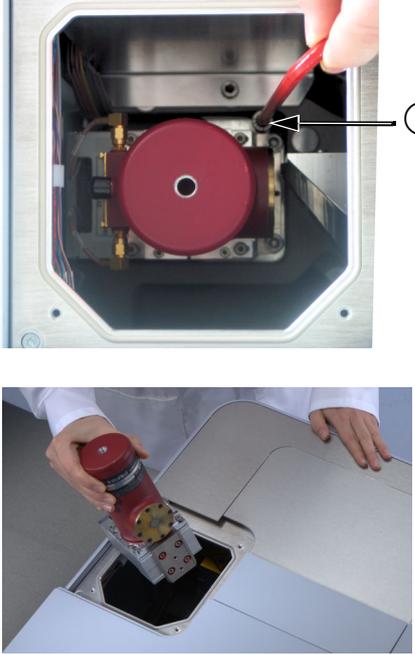
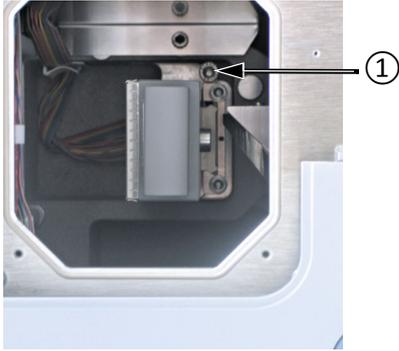
Make sure that the spectral range of the installed optical spectrometer components (source, beamsplitter, detector and sample compartment windows, if installed) correspond with each other! (See also section 5.9.)

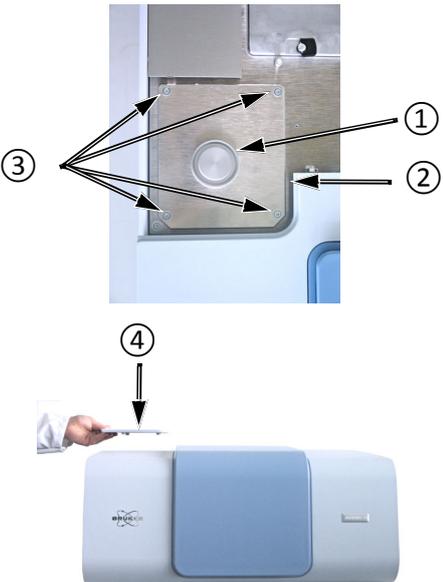
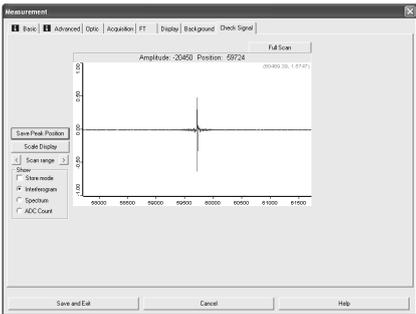
5.11.2 Procedure

	<p>Required tools</p> <ul style="list-style-type: none"> • TORX screw driver <p>Note: This tool is included in the delivery scope of the spectrometer.</p> <ul style="list-style-type: none"> • Hex key (size: 6 mm) <p>Note: This tool is included in the delivery scope of the DigiTect-type detector.</p>
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The optionally available detectors are mounted on a dovetail slide which allows an easy exchange. A re-alignment is not necessary.

<p>1</p>		<p>To gain access to the detector:</p> <p>1. Remove the plastic cover ①.</p> <p>Note: This cover is held in place magnetically.</p> <p>2. Loosen the four TORX screws ② and remove the metallic cover ③.</p>
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<p>2</p>		<p>To remove the detector:</p> <ol style="list-style-type: none"> 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. <p>Caution: Remove the detector carefully in order not to damage the detector and/or the mirrors which are installed in the detector compartment.</p>
<p>3</p>		<p>To install the exchange detector:</p> <ol style="list-style-type: none"> 1. Insert the exchange detector precisely into the dovetail guide and push the detector downwards until you feel a resistance. <p>Caution: Insert the detector carefully in order not to damage the detector and/or the mirrors which are installed in the detector compartment.</p> <ol style="list-style-type: none"> 2. Fasten the Allen screw ① using the supplied hex key (size 6mm). <p>➤ A beep indicates that the detector has been recognized by the electronics. The electrical connections are established automatically.</p>

<p>4</p>		<p>To close the spectrometer:</p> <p>Note: In case an MCT detector is installed, the blind cap ① needs to be removed first.</p> <ol style="list-style-type: none"> 1. Put the metallic cover ② in place and fasten the four screws ③. 2. Put the plastic cover ④ in place. <p>Note: This cover is held in place magnetically. Ensure that it is positioned correctly.</p>
<p>5</p>		<p>To check the signal:</p> <p>Open the OPUS software program and check whether a signal is detected and whether the signal intensity is OK.</p> <p>☞ For information about how to check the signal, see section 5.13.</p>

5.12 Replacing a sample compartment window

5.12.1 General information

The sample compartment windows need to be replaced in the following cases:

- for changing the spectral range
- the window is broken or opaque¹

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

5.12.2 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.

5.12.3 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

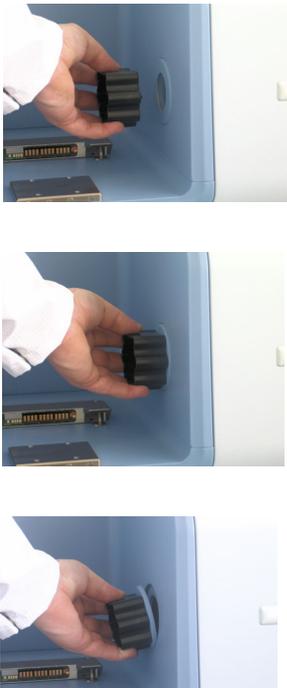
Non-observance of the following safety instructions could result in death or serious injury.

- 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 instructions of the attached safety data sheets.



1. If the opaqueness has reached such a degree that the transparency (infrared transmittance) is seriously reduced, the window needs to be replaced. Especially windows made of hygroscopic material tend to become opaque in the course of time. For an overview about the available window materials and their properties, see section 4.5.5.

5.12.4 Replacement procedure

	<p>Required tool</p> <p>Special tool for removing / installing a window or flange</p> <p>Note: This tool is included in the delivery scope of the spectrometer.</p>
<p>1</p>	 <p>Open the large-sized sample compartment.</p>
<p>2</p>	<p>Remove the window assembly:</p> <p>Position the tool with the label TOP pointing upwards.</p> <p>Insert the pins of the tool into the corresponding holes of the window assembly.</p> <p>Note: The tool is attracted magnetically to the window assembly.</p> <p>Slightly rotate the tool to overcome the magnetic attractive force.</p> 
<p>3</p>	<p>Reinstall the window assembly:</p> <p>Insert the pins of the tool into the corresponding holes of the window assembly.</p> <p>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.</p> <p>The window assembly is attracted magnetically to the sample compartment wall.</p> <p>➤ A beep indicates that the window has been recognized by the electronics.</p> 

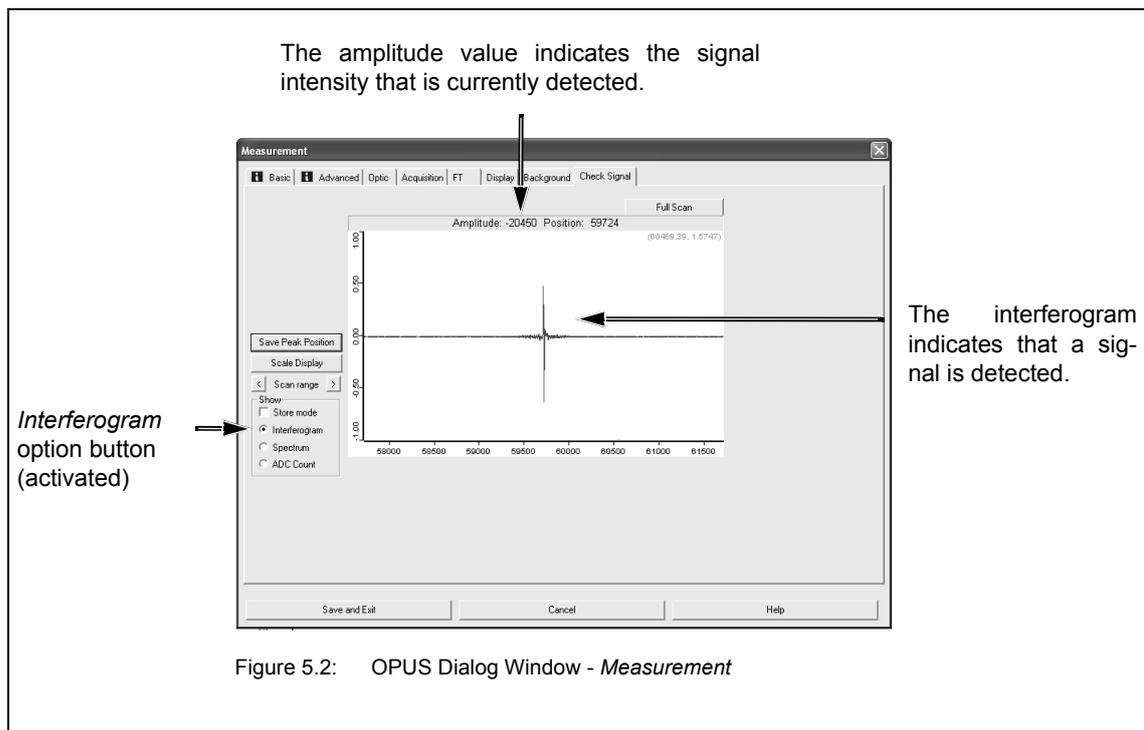
5.13 Checking the signal

5.13.1 General information

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

5.13.2 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. 5.2.)



For verifying the currently detected signal intensity, compare the amplitude value displayed in OPUS (fig. 5.2) with the amplitude value stated in the supplied OQ test protocol¹. (See fig. 5.3.)

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.



Figure 5.3: OQ- Test Protocol

If there is not any signal detected or if the amplitude value displayed in OPUS (fig. 5.2) deviates significantly from amplitude value of the supplied OQ test protocol (fig. 5.3) check the installation of the spectrometer component(s) you have replaced before. For troubleshooting, see also section .7.5.4

5.13.3 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. 5.4), you have to save the new peak position.

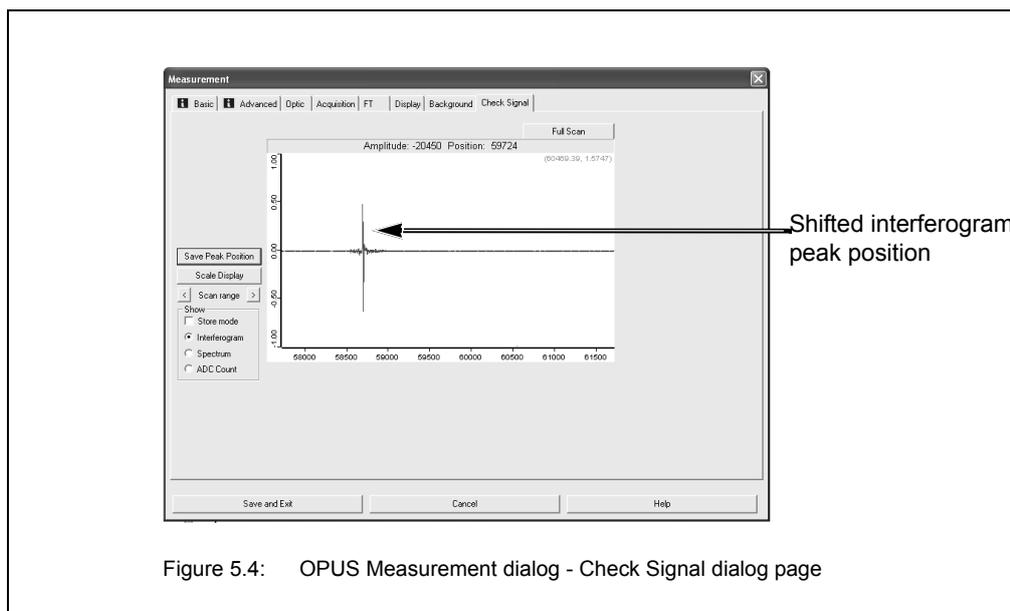


Figure 5.4: OPUS Measurement dialog - Check Signal dialog page

- 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.

5.14 Cooling a detector with liquid nitrogen

5.14.1 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 5.13.

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.

5.14.2 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.

5.14.3 Preparing the detector compartment cover for funnel insertion

General information

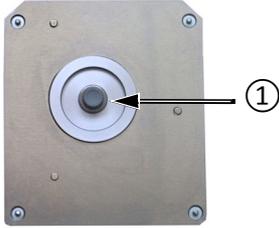
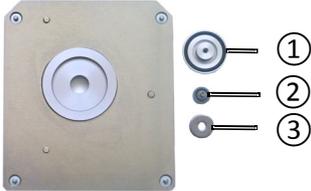
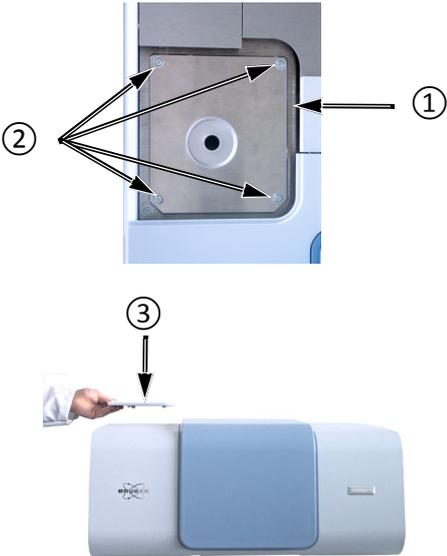
In case the liquid nitrogen-cooled detector has been delivered together with the spectrometer, the detector compartment cover is already prepared for the funnel insertion. If the detector has been ordered at a later date you need to prepare the detector compartment cover as described below.

Required tool

	<p>Required tool</p> <ul style="list-style-type: none"> • TORX screw driver <p>Note: This tool is included in the delivery scope of the spectrometer.</p>
---	---

Procedure

<p>1</p>		<p>To gain access to the detector:</p> <ol style="list-style-type: none"> 1. Remove the plastic cover ①. <p>Note: This cover is held in place magnetically.</p> <ol style="list-style-type: none"> 2. Loosen the four TORX screws ② and remove the metallic cover ③. <p>Required tool: TORX screw driver</p>
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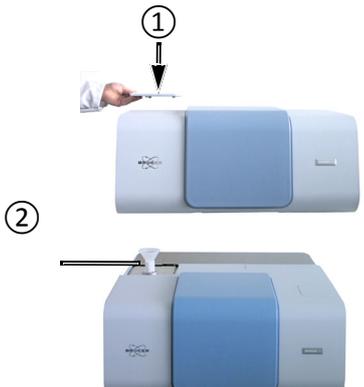
2		<p>Turn the detector compartment cover upside down and remove the cap from the filling hole.</p> <p>To do this, screw off the knurled screw ① and remove the complete closure assembly.</p>
		<p>The closure assembly consists of the following items:</p> <ul style="list-style-type: none"> ① - cap ② - knurled screw ③ - washer
3		<p>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!</p> <p>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.</p>
4		<p>1. Put the metallic cover ① in place and fasten the four TORX screws ②.</p> <p>2. Put the plastic cover ③ in place.</p> <p>Note: This cover is held in place magnetically. Ensure that it is positioned correctly.</p>

5.14.4 Filling liquid nitrogen into the detector

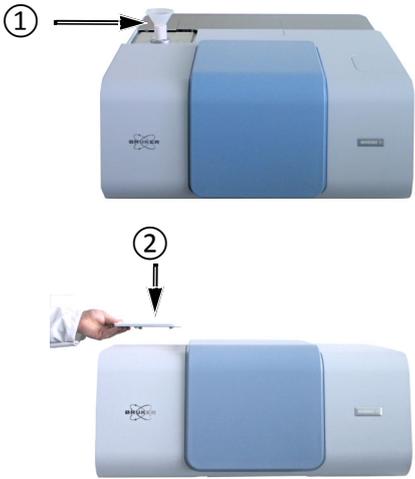
Required equipment and consumables

- 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

<p>1</p>		<p>1. Remove the plastic cover ①.</p> <p>Note: This cover is held in place magnetically.</p> <p>2. Insert the funnel ②.</p>
<p>2</p>		<p>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.</p> <p>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.</p> <p>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.</p> <p>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:</p> <ul style="list-style-type: none"> ➤ 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.

Operation 5

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

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



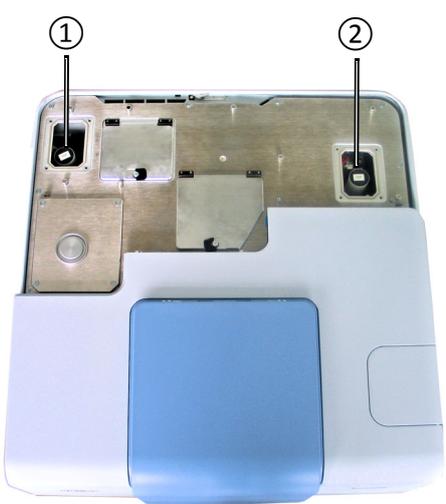
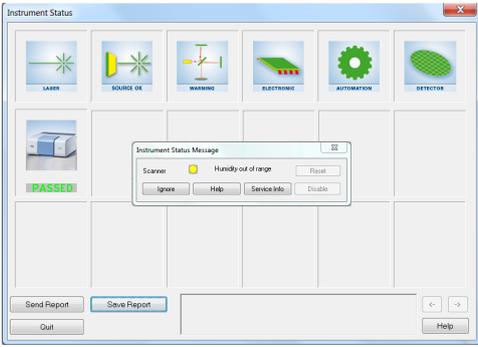
Damage to ESD-sensitive electronic spectrometer components because of accidental electrostatic discharges (ESD)

- > 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.

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

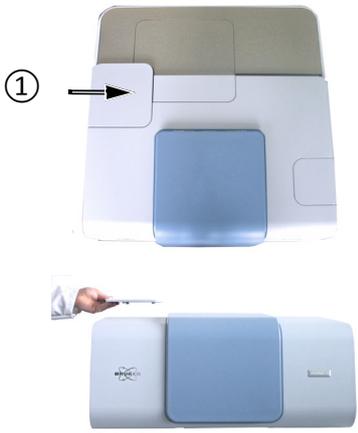
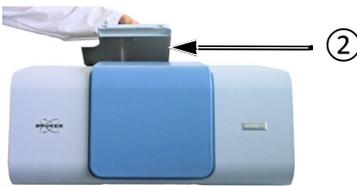
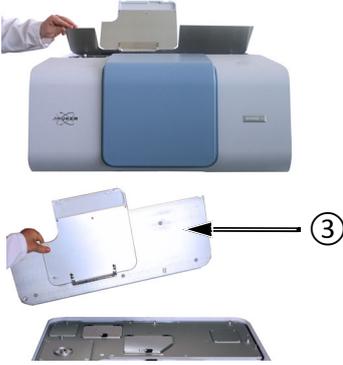
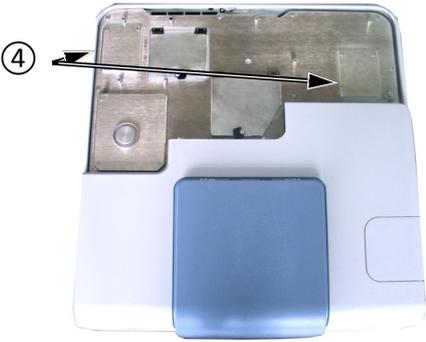
You can either regenerate the desiccant as described in section 6.2.4 and reuse it or order a new desiccant cartridge. (For the order number refer to section B.1.)

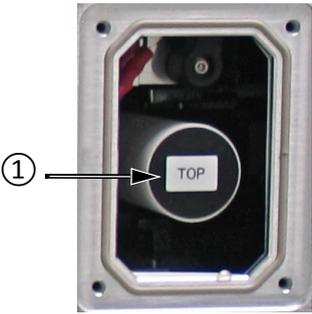
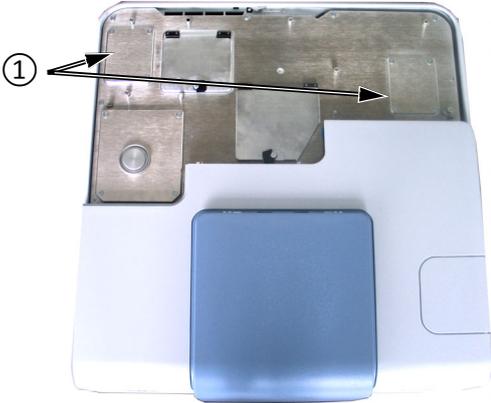
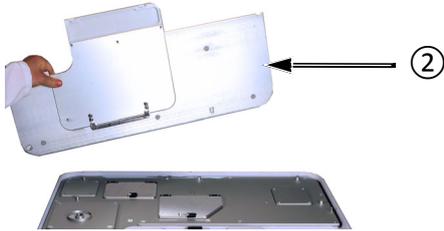
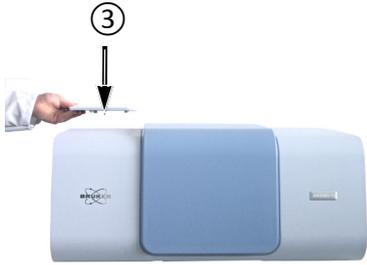
6.2.2 Storage notes

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

	<p>Required tool</p> <ul style="list-style-type: none"> • TORX screw driver <p>Note: This tool is included in the delivery scope.</p>
<p>1</p>	<div data-bbox="400 510 758 943">  </div> <div data-bbox="469 987 826 1173">  </div> <div data-bbox="456 1234 799 1599">  </div> <div data-bbox="360 1653 786 1995">  </div> <div data-bbox="903 499 1412 2022"> <p>To gain access to the desiccant cartridges:</p> <ol style="list-style-type: none"> 1. Remove the plastic cover (1) which provides access to the DigiText detector. <p>Note: This cover is held in place magnetically.</p> <ol style="list-style-type: none"> 2. Fold back the outer lid (2) to facilitate the removal of the metallic cover. <ol style="list-style-type: none"> 3. Remove the metallic cover (3). <ol style="list-style-type: none"> 3. Remove the two lids (4) which provide access to the desiccant cartridges by loosening the four TORX screws at each lid. <p> 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.</p> </div>

<p>2</p>		<p>To replace the desiccant cartridge:</p> <p>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.</p>
<p>3</p>		<p>To close the spectrometer:</p> <p>1. Reinstall the two lids ① by fastening the four screws at each lid.</p>
		<p>2. Put the metallic cover ② back in place.</p> <p>Note: The cover is held in place magnetically. Ensure that it is positioned correctly.</p>
		<p>3. Put the plastic cover ③ back in place.</p> <p>Note: This cover is held in place magnetically. Ensure that it is positioned correctly.</p>

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 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 times¹: 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.

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.

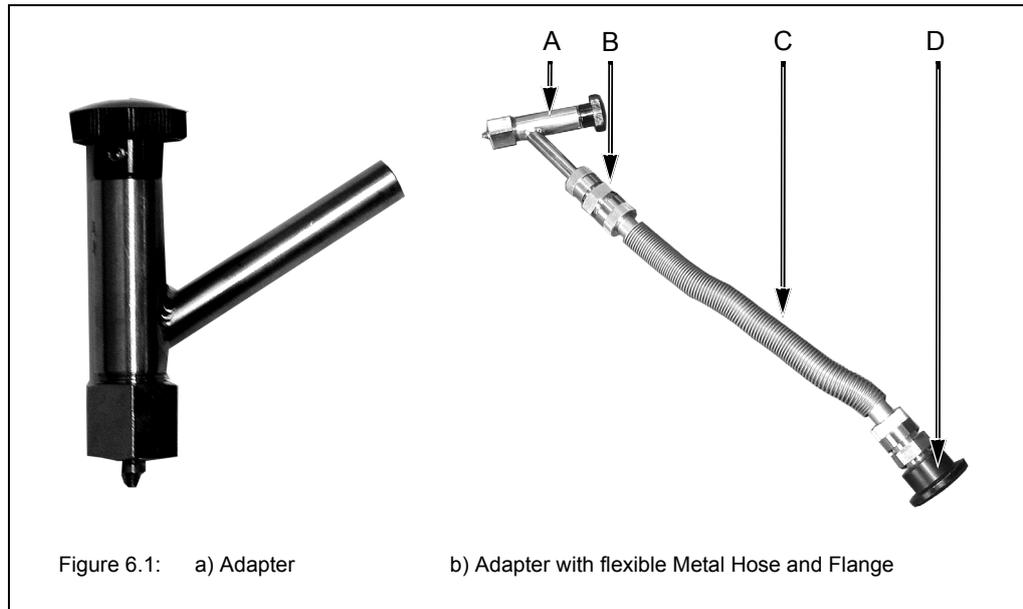
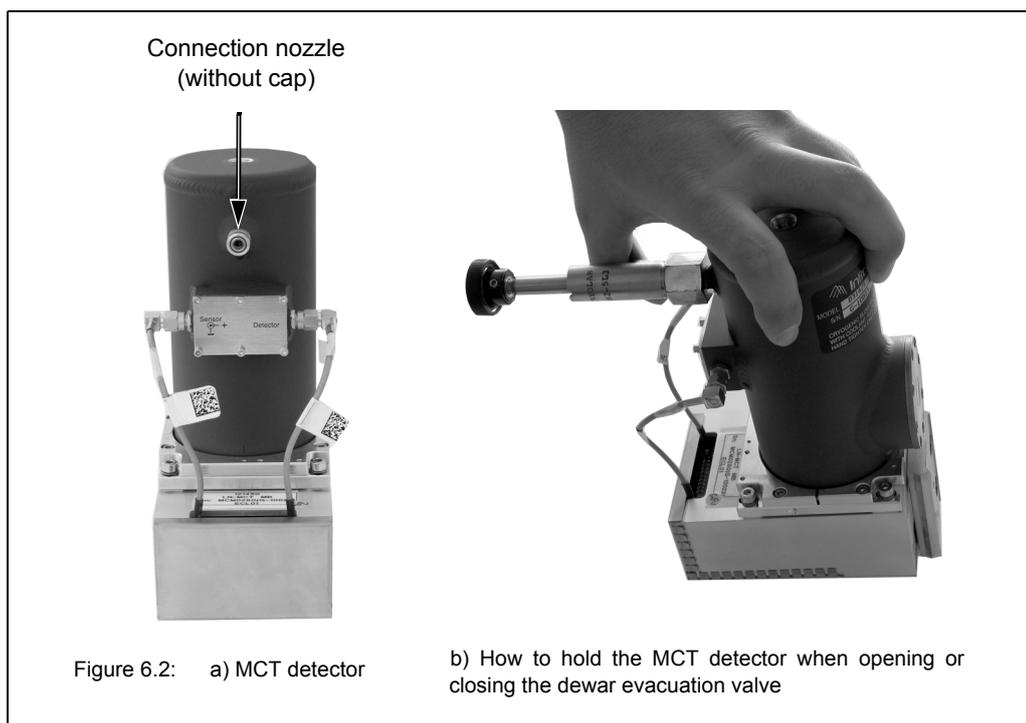


Fig. 6.1	Component
A	Connecting adapter (for connecting the vacuum pump to the detector dewar)
B	Flange
C	Flexible metal hose
D	NW 25 flange (for connecting to the vacuum pump)

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 5.11.2.
- 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).



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 5.11.2.
- 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.

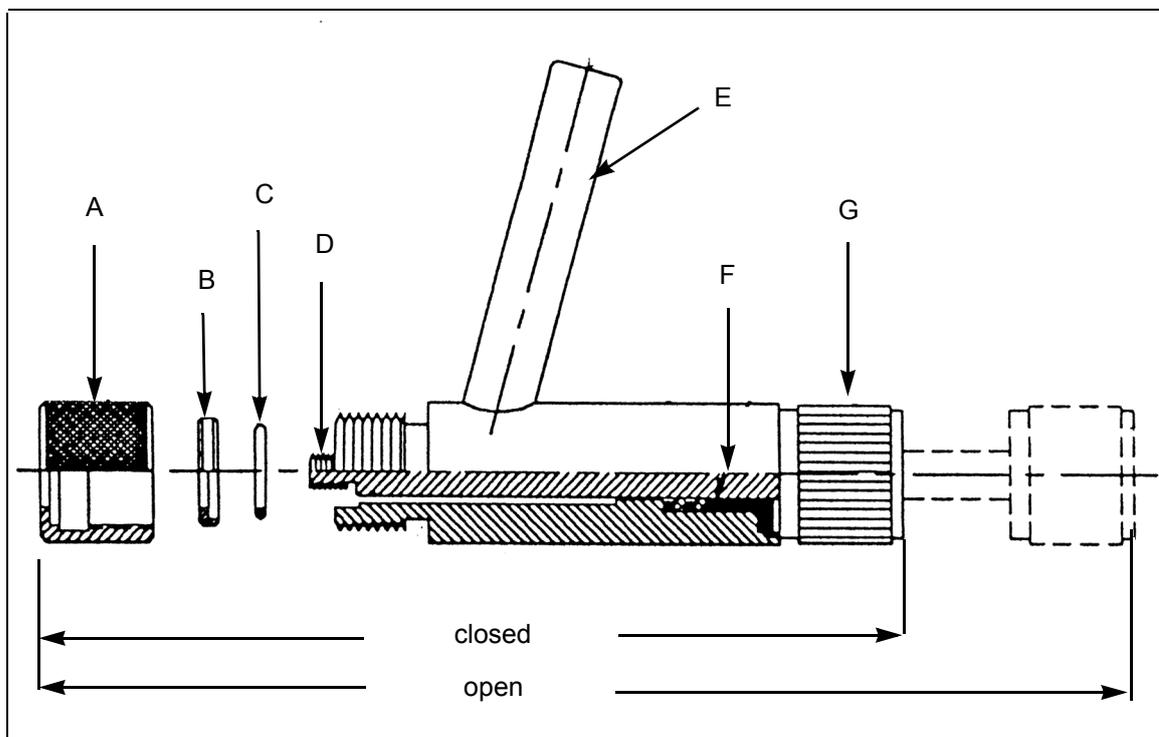


Figure 6.3: Connecting adapter - Cross section

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

In case a sample compartment window has got broken or its opaqueness¹ has reached such a degree that the transparency (infrared transmittance) is seriously reduced, it needs to be replaced.

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. In this case, observe the following safety notes:

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.



When installing a new sample compartment window, make sure that its transmission range corresponds with the spectral range of the other installed spectrometer components: source, beamsplitter and detector. (See also section 2.2.)

- ☞ For the order number of the sample compartment windows, refer to section B.3.
- ☞ For information about the replacement procedure and handling instructions, refer to section 5.12.

6.5 Performing an OQ test² with OVP³

After the replacement of a defective optical component⁴, it is highly recommended to perform an OQ test for the test channels in question to ensure that the spectrometer achieves the specified parameter values⁵.

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.

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.
2. OQ test - Operational Qualification Test
3. OVP - Opus Validation Program is intended for performing spectrometer validation tests like OQ and PQ. It is an integral part of the OPUS software.
4. 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.
5. 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.

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.)

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)

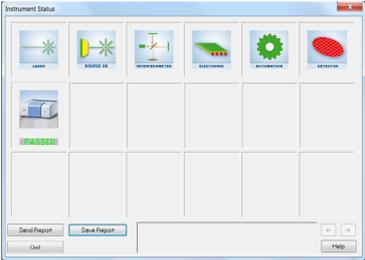
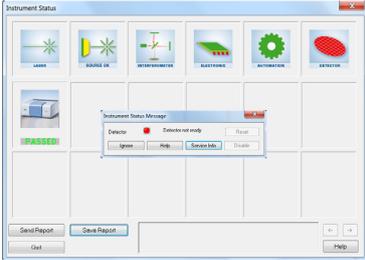
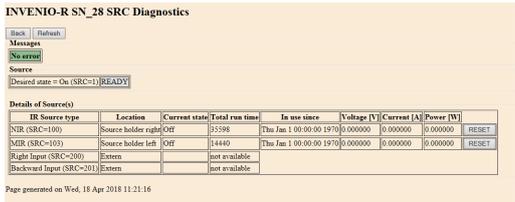
The available diagnostic means (e.g. spectrometer status indicator LED, instrument status messages in OPUS, diagnostics pages of the spectrometer firmware) enable the operator to identify many spectrometer problems, or at least to narrow down a problem.

☞ 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.

Due to easy-to-replace spectrometer components, the operator can solve many problems himself. The holders and/or locking mechanisms for the spectrometer components beamsplitter and DigiTect-type detector ensure a correct installation position of these components, i.e. after the replacement of these components, a realignment is not required.

7.2 Diagnostic means

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

	<p>Spectrometer status indicator (LED strip ①) below the large-sized sample compartment</p> <p>☞ See section 7.2.1</p>																																													
	<p>OPUS dialog window <i>Instrument Status</i></p> <p>☞ See section 7.2.2.</p>																																													
	<p>Instrument status messages in OPUS</p> <p>☞ See section 7.2.3.</p>																																													
 <p>INVENIO-R SN_28 SRC Diagnostics</p> <p>Back Refresh</p> <p>Messages</p> <p>Message</p> <p>Source</p> <p>Desired state = On (SRC=1) READY</p> <p>Details of Source(s)</p> <table border="1"> <thead> <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> </thead> <tbody> <tr> <td>NIR (SRC=100)</td> <td>Source holder right</td> <td>OFF</td> <td>33598</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=100)</td> <td>External</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Backward Input (SRC=201)</td> <td>External</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> </tbody> </table> <p>Page generated on Wed, 18 Apr 2019 11:21:16</p>	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	33598	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=100)	External								Backward Input (SRC=201)	External								<p>Diagnostics pages of the spectrometer firmware</p> <p>☞ See section 7.2.4.</p>
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	33598	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=100)	External																																													
Backward Input (SRC=201)	External																																													

7.2.1 Spectrometer status indicator

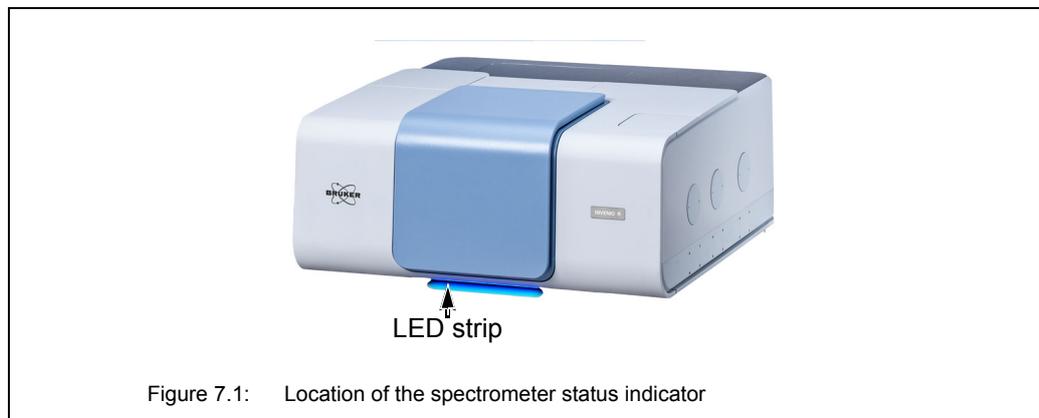


Figure 7.1: Location of the spectrometer status indicator

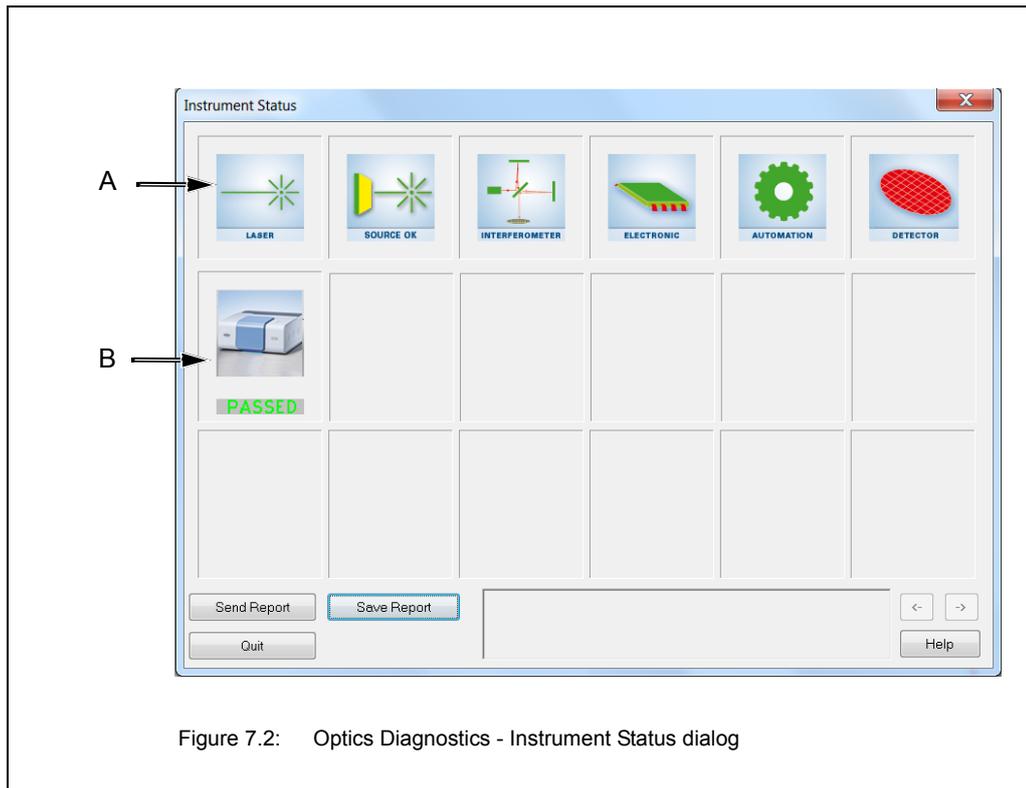
Below the large sample compartment, there is a LED strip which indicates the current spectrometer status. The color of the LEDs give a general indication of the operating status of the spectrometer.

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: <ul style="list-style-type: none"> • 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: <ul style="list-style-type: none"> • 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. <p>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.</p> <p>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.</p> <p>☞ See section 7.5.2 for troubleshooting.</p>
LEDs light up red.	A red instrument status LED indicates an error. For example, this is the case when: <ul style="list-style-type: none"> • an optical component (e.g. NIR source, laser) fails or does not achieve its performance specification <p>Note: In case the instrument status LED lights red, measuring is not possible until the cause of the error is eliminated.</p> <p>☞ See section 7.5.1 for troubleshooting.</p>

7.2.2 OPUS dialog *Instrument Status*

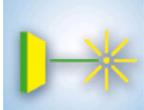
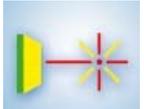
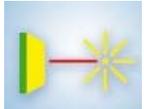
The OPUS dialog window *Instrument Status* allows you to diagnose which spectrometer component has caused the failure or to find out whether an OVP test¹ has expired or failed. To perform a fault diagnosis, proceed as follows:

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



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:

 <p>SOURCE OK</p>	<p>OK Component is okay.</p>
 <p>SOURCE WARNING</p>	<p>WARNING The exact meaning of a warning depends on the component in question. For example, in case of the source, a warning means:</p> <ul style="list-style-type: none"> • End of the specified lifetime of the component is nearly reached. In this case, measuring is still possible. <p>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.</p>
 <p>SOURCE ERROR</p>	<p>ERROR Component is defective. In case of an error, measuring is no longer possible.</p>

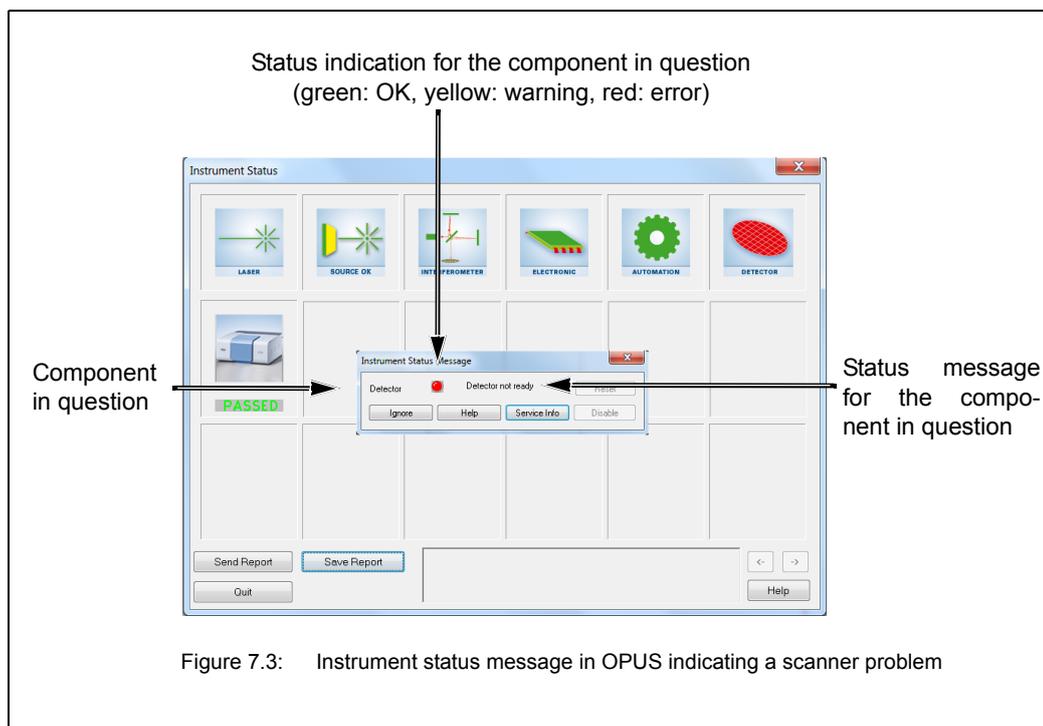
- B) The second row of icons refers to the possible active test channels and indicates the result of the last OVP test performed. The results can be as follows:

	<p>PASSED (green): OVP test passed. Test is still valid.</p>
	<p>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.)</p>
	<p>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.</p>
	<p>INACTIVE (yellow): This test channel has been set up but no OVP test has been performed yet and all OVP tests are disabled.</p>

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.



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.

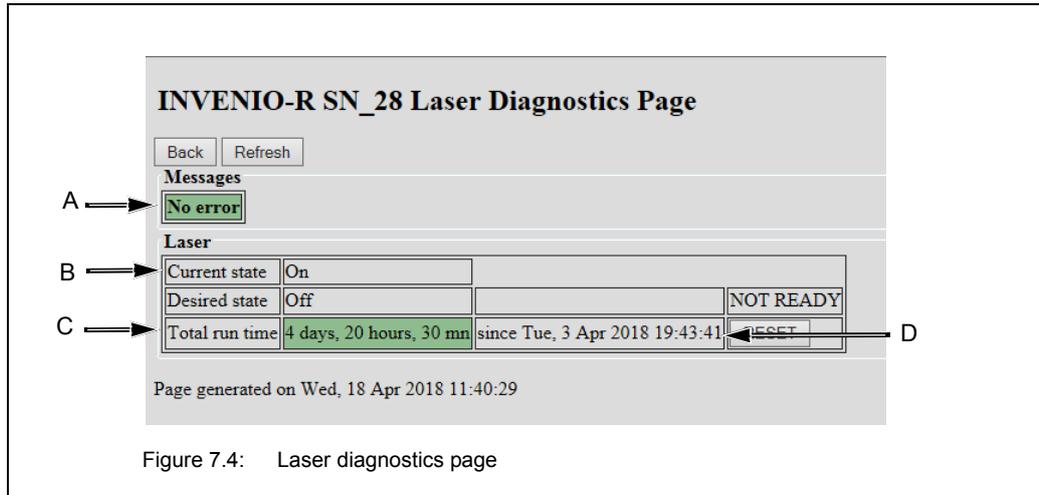


Figure 7.4: Laser diagnostics page

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

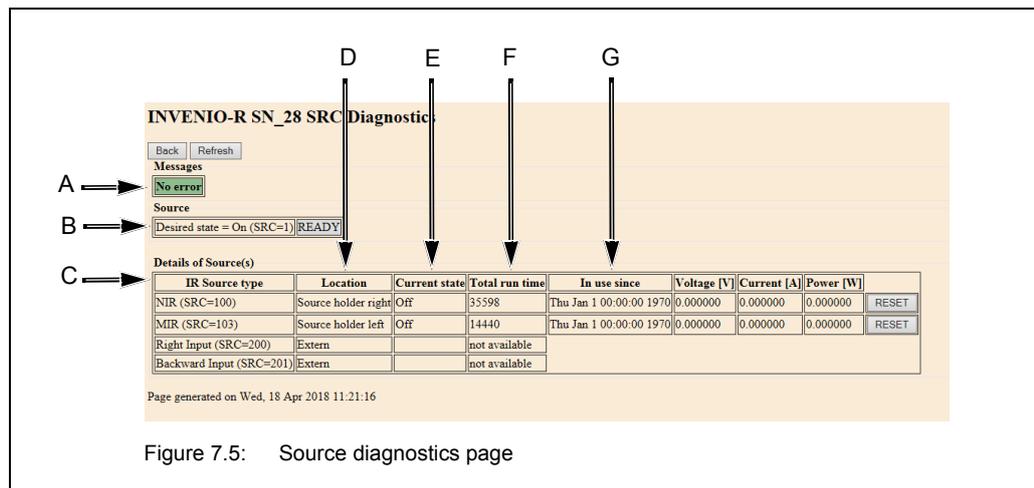


Figure 7.5: Source diagnostics page

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-R SN_28 Scanner Diagnostics

Back Refresh Auto-Reload

Messages

A → **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.

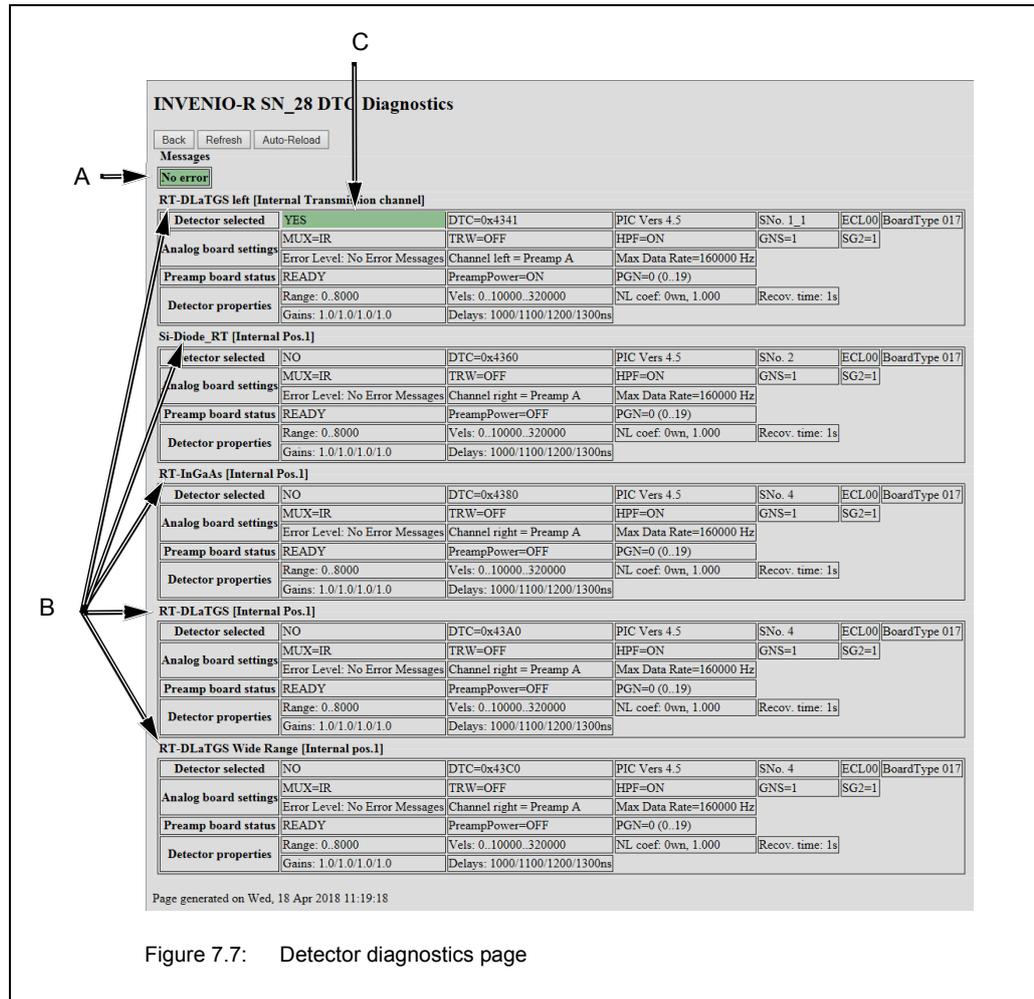


Figure 7.7: Detector diagnostics page

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.

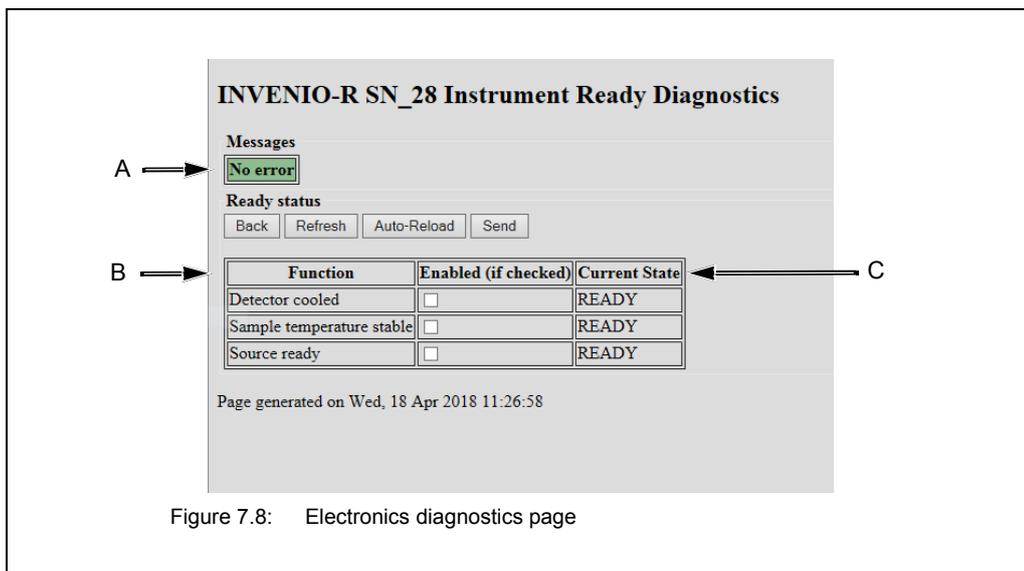


Figure 7.8: Electronics diagnostics page

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

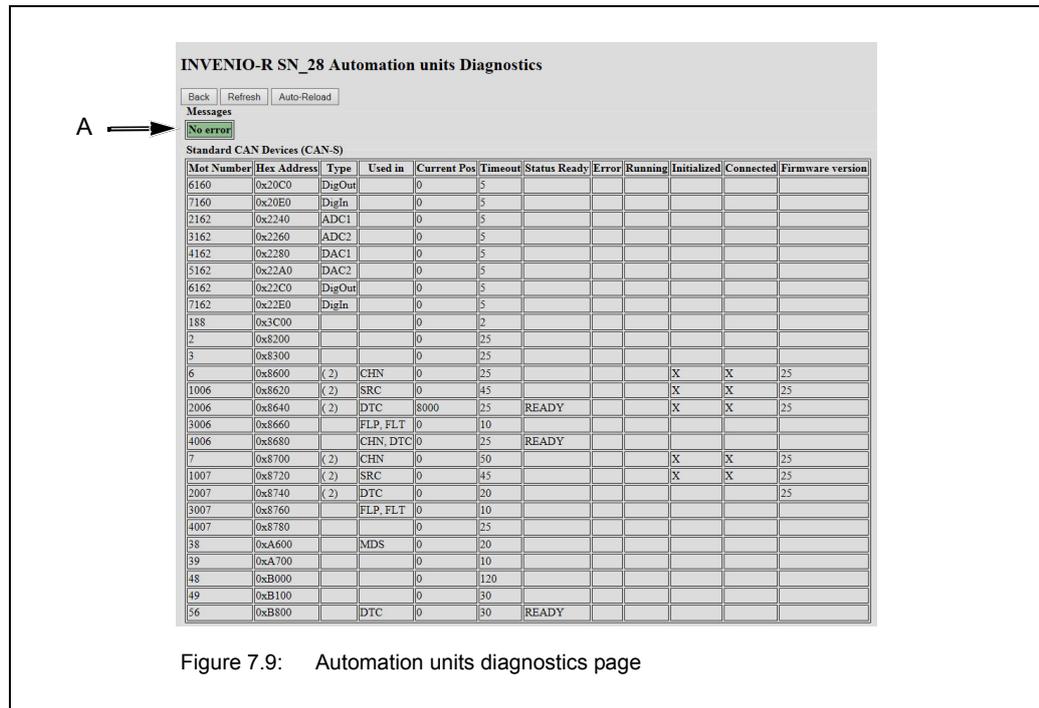


Figure 7.9: Automation units diagnostics page

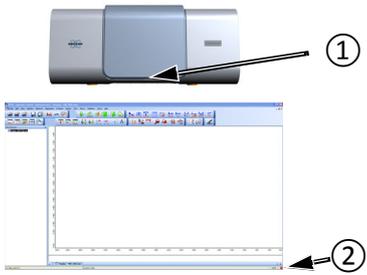
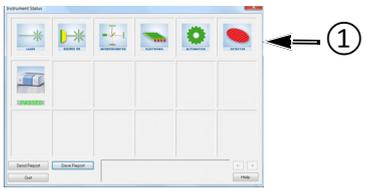
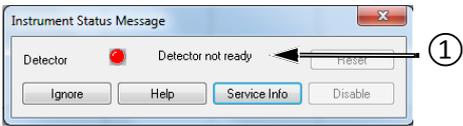
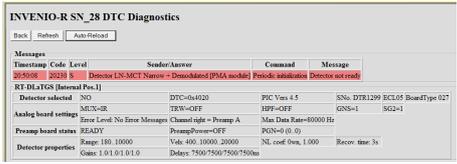
Fig. 7.9	Explanation
A	Possible error message Note: They are identical to the instrument status message in OPUS.

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 5.13.)
- 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		<p>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.</p> <p>➤ Are they red or yellow?</p>
2		<p>If so, open the OPUS dialog window <i>Instrument Status</i> and check whether there is a component having the status WARNING or ERROR.</p>
3		<p>If so, double-click on the component icon in question to look up whether an instrument status message ① is displayed in OPUS.</p> <p>🔍 For information about the meaning of the instrument status messages refer to section 7.5.3.</p>
4		<p>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.</p> <p>🔍 See section 7.2.4.</p>

🔍 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

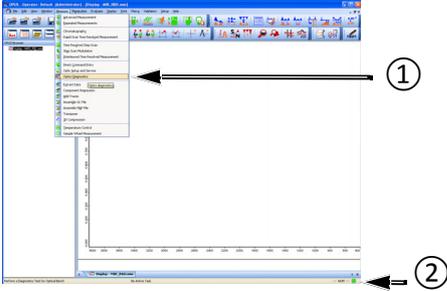
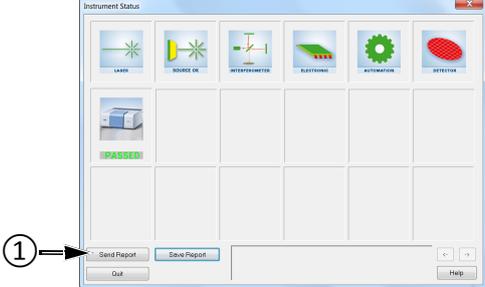
Remote fault diagnosis means that you send a complete spectrometer status report - a so called *Full Report* - by e-mail to Bruker. This report enables a Bruker service technician to perform a first remote fault diagnostics.

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:

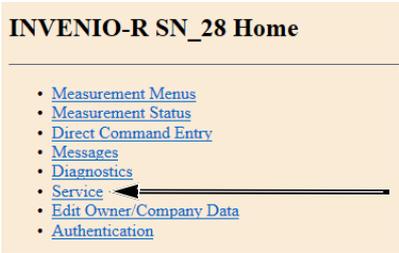
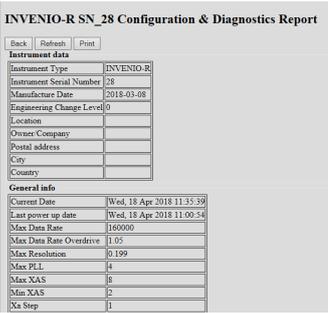
1		<p>Open the OPUS software program, if not already done.</p> <p>Either select in the OPUS <i>Measure</i> menu the <i>Optics Diagnostics</i> function ① or click on the OPUS status light ②.</p> <p>➤ Thereupon, the <i>Instrument Status</i> dialog opens.</p>
2		<p>Click on the <i>Send Report</i> button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

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		<p>Open an Internet browser. Enter the spectrometer IP address in the Internet browser entry field ① and press the ENTER key.</p> <ul style="list-style-type: none"> • 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-r-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.
2		<p>➤ Thereupon, the spectrometer home page opens.</p> <p>Click on <i>Service</i> ①.</p>
3		<p>Click on <i>Full Report</i> ①.</p>
4		<p>Save the full report as *.htm file for sending it as an e-mail attachment.</p> <p>Send the full report by e-mail as an attached file to <i>opusreports@bruker.com</i>.</p>

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. NIR 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
<p>If the laser is the cause of the problem either:</p> <ul style="list-style-type: none"> • the laser is defective or • the laser is improperly installed. <p>➤ Note: These causes are also indicated by the instrument status message: <i>HeNe-Laser is off or no laser signals</i>.</p> <p>➤ Note: The laser has a limited service lifetime of about 25,000 operating hours. Look up the actual service lifetime of the installed laser at the <i>Laser Diagnostics Page</i>. See fig. 7.4.)</p>	<p>Improperly installed laser: Check whether the laser is installed properly and correct it, if required.</p> <p>Defective laser: Order a replacement laser. For the order number refer to section B.1. After receiving the replacement laser, replace the defective component.</p> <p>☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Laser Replacement Instructions</i> which is added to the replacement laser.</p> <hr/> <p>i Replacing the laser is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>

Possible causes	Solutions
<p>If the source is the cause of the problem either:</p> <ul style="list-style-type: none"> • the selected source is defective or • the selected source is not or not properly installed. <p>➤ Note: This problem is indicated by the instrument status message <i>Source is broken or not connected</i>.</p>	<p>Missing source: Install the source.</p> <p>Improperly installed source: Check whether the source is installed properly and correct it, if required.</p> <p>Defective source: Order a replacement source. For the order number refer to section B.1. After receiving the replacement source, replace the defective source.</p> <p>☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Source Replacement Instructions</i> which is added to the replacement source.</p> <hr/> <p>i Replacing the source is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>
<p>If the detector is the cause of the problem:</p> <ul style="list-style-type: none"> • the detector is defective: This problem is indicated by the instrument status message <i>Device not connected. No analog board selected</i>. • the MCT detector is not cooled down to its operating temperature. This problem is indicated by the instrument status message <i>Detector not ready</i>. • the optional DigiTect-type detector is not properly installed: This problem is indicated by the instrument status message <i>Device not connected. No analog board selected</i>. 	<p>Defective detector: Contact the Bruker service.</p> <p>☞ For the Bruker service contact data, see section 1.6.</p> <p>MCT detector temperature is too high: Fill liquid nitrogen into the MCT detector dewar.</p> <p>☞ See section 5.14.</p> <p>Improperly installed DigiTect-type detector: Check whether the detector is installed correctly and correct it, if required. See section 5.11.</p>
<p>If the interferometer (scanner) is the cause of the problem there are a number of possible causes. For example:</p> <ul style="list-style-type: none"> • The beamsplitter is not locked. <p>➤ Note: This problem is indicated by the instrument status message <i>BMS door is open</i>.</p>	<p>Unlocked beamsplitter: Lock the beamsplitter.</p> <p>☞ See section 5.10.2.</p> <p>In case of a different cause, try to narrow down the trouble source by consulting the <i>Scanner Diagnostics Page</i>. (See fig. 7.6.) For error messages regarding the interferometer, see section 7.5.3.3.</p> <p>If you can not solve the problem, contact the Bruker service.</p> <p>☞ For the Bruker service contact data, see section 1.6.</p>

Possible causes	Solutions
<p>If the automation is the cause of the problem there are a number of possible causes.</p>	<p>Try to narrow down the trouble source by consulting the <i>Automation Units Diagnostics Page</i>. (See fig. 7.9.)</p> <p>If you can not solve the problem, contact the Bruker service.</p> <p>☞ For the Bruker service contact data, see section 1.6.</p>
<p>If the electronics is the cause of the problem there are a number of possible causes. For example:</p> <ul style="list-style-type: none"> • the electronics unit is defective or • there is a short circuit. 	<p>Defective power supply unit: Contact the Bruker service.</p> <p>☞ For the Bruker service contact data, see section 1.6.</p> <p>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.</p> <p>☞ For the Bruker service contact data, see section 1.6.</p>

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
<p>Water vapor concentration inside the spectrometer is too high.</p> <p>Note: In this case, the instrument status message <i>Humidity out of range</i> is displayed in OPUS.</p>	<p>In general, the following actions can solve the problem:</p> <ul style="list-style-type: none"> • 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.
<p>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.</p> <p>🔗 See section 7.2.2.</p>	<p>Perform the PQ or OQ test for the currently selected measurement channel.</p> <p>🔗 For detailed information about OVP refer to the OPUS Reference Manual.</p>

Possible causes	Solutions
<p>The end of the specified lifetime of the source and/or laser is nearly reached.</p>	<p>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: <i>End of the average lifetime is nearly reached, spare part will be required.</i></p> <ul style="list-style-type: none"> ☞ See section 7.2.2 and section 7.2.3. <p>Order the corresponding replacement part. For the order number refer to section B.1. After receiving the replacement part, replace it.</p> <ul style="list-style-type: none"> ☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Source Replacement Instructions</i> or the document <i>INVENIO - Laser Replacement Instructions</i> which is added to the replacement part. <hr/> <p>i Replacing the laser / source is a recommended Bruker service delivery.</p> <hr/> <ul style="list-style-type: none"> ☞ 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 <i>Ignore</i> button in the <i>Instrument Status Message</i> 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
<p>HeNe laser is off or no laser signal.</p>	<p>Laser tube is not orientated correctly. OR Power supply to the laser is interrupted. OR Laser is defective.</p>	<p>Improperly installed laser: Check whether the laser is installed properly and correct it, if required.</p> <p>Defective laser: Order a replacement laser. For the order number refer to section B.1. After receiving the replacement laser, replace the defective component.</p> <p>☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Laser Replacement Instructions</i> which is added to the replacement laser.</p> <hr/> <p>i Replacing the laser is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>

Instrument status message	Possible causes	Solutions
<p>End of average lifetime is nearly reached, spare part will be required.</p>	<p>The end of the specified lifetime of the laser is nearly reached.</p> <p>Note: If this message is displayed, first find out of which component - laser or source - the specified lifetime is nearly reached.</p>	<p>The laser needs to be replaced in the near future.</p> <p>Order a replacement laser. For the order number refer to section B.1. After receiving the replacement laser, replace it.</p> <ul style="list-style-type: none"> ☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Laser Replacement Instructions</i> which is added to the replacement laser. <hr/> <p>i Replacing the laser is a recommended Bruker service delivery.</p> <hr/> <ul style="list-style-type: none"> ☞ 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 <i>Ignore</i> button in the <i>Instrument Status Message</i> 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.	<p>Source is not installed at all or not installed properly.</p> <p>OR</p> <p>Source is defective (e.g. burnt out).</p>	<p>Install the source properly.</p> <p>Order a spare source. For the order number refer to section B.1. After receiving the replacement source, replace it.</p> <p>☞ For information about the proper installation and the replacement procedure, see the added document <i>INVENIO - Source Replacement Instructions</i>.</p> <hr/> <p>i Replacing the source is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>
End of average lifetime is nearly reached, spare part will be required.	<p>The end of the specified lifetime of the source is nearly reached.</p> <p>Note: If this message is displayed, first find out of which component - laser or source - the specified lifetime is nearly reached.</p>	<p>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.</p> <p>☞ For information about the proper installation and the replacement procedure, see the added document <i>INVENIO - Source Replacement Instructions</i>.</p> <hr/> <p>i Replacing the source is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>

Instrument status message	Possible causes	Solutions
		<ul style="list-style-type: none"> ➤ Note: Despite this warning message, measuring is still possible. To turn the OPUS status light green again click on the <i>Ignore</i> button in the <i>Instrument Status Message</i> 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
BMS door is open.	Beamsplitter is not installed properly (i.e. the beamsplitter is not in the locked position).	Lock the beamsplitter in position. ⓘ See section 5.10.2.
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.	<p>In general, the following actions can solve the problem:</p> <ul style="list-style-type: none"> • 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.	<p>Cool down the MCT detector by filling liquid nitrogen into the detector dewar.</p> <p>☞ See section 5.14.</p>
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.	<p>Install the detector.</p> <p>☞ See section 5.11.</p>

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 thermoelectrically cooled detector, the detector temperature is too high. ➤ This problem is indicated by the instrument status message <i>Detector not ready</i> .	MCT detector: Cool the MCT detector with liquid nitrogen. ☞ See section 5.14. Thermoelectrically 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 <i>Device not connected. No analog board selected</i> .	Internal detectors (optional DigiTect-type detector): Install the detector properly. ☞ See section 5.11. 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 <i>Measurement</i> , dialog page <i>Optics</i> . See section C.2.
Source is not or not properly installed or it is defective. ➤ These problems are indicated by the instrument status message <i>Source is broken or not connected</i> .	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 <i>INVENIO - Source Replacement Instructions</i> . i Replacing the source is a recommended Bruker service delivery. ☞ For the Bruker service contact data, see section 1.6.

Possible Causes	Solutions
<p>Beamsplitter is not locked in position.</p> <p>➤ This problem is indicated by the instrument status message <i>BMS door is open</i>.</p>	<p>Lock the beamsplitter in position.</p> <p>☞ See section 5.10.2.</p>
<ul style="list-style-type: none"> • 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. Especially hygroscopic materials (e.g. CsI, KBr) tend to become opaque. • Beamsplitter is dirty or damaged. 	<p>Order a replacement beamsplitter. For the order number refer to section B.2. After receiving the replacement beamsplitter, replace it.</p> <p>☞ See section 5.10.2.</p>
<p>Beamsplitter is not properly installed.</p> <p>➤ This problem is indicated by the instrument status message <i>NOT SCANNING. Laser-A modulation too small, Laser-B modulation too small, Laser signal modulation is too small</i>.</p>	<p>Install the beamsplitter properly.</p> <p>☞ See section 5.10.2.</p>
<p>A temporary or permanent optics misalignment caused by strong shock.</p>	<p>Place the spectrometer on a vibration-free surface. In case of a temporary optics misalignment, this action can solve the problem.</p> <p>If this action does not solve the problem contact the Bruker service.</p> <p>☞ For the Bruker service contact data, see section 1.6.</p>
<p>If the laser is the cause of the problem either:</p> <ul style="list-style-type: none"> • the laser beam is blocked (e.g. due to an improperly installed laser) or • the laser power supply cable is not connected and/or secured properly or • the laser is defective. <p>➤ These causes are also indicated by a red spectrometer status LED and by the instrument status message: <i>HeNe-Laser is off or no laser signals</i>.</p>	<p>Improperly installed laser: Check whether the laser is installed properly and correct it, if required.</p> <p>Defective laser: Order a replacement laser. For the order number refer to section B.1. After receiving the replacement laser, replace the defective component.</p> <p>☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Laser Replacement Instructions</i> which is added to the replacement laser.</p> <hr/> <p>i Replacing the laser is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>

7.5.5 A failed validation test

Validation test is a collective term for all tests (e.g. OQ test¹, PQ test²) that can be performed with OVP³ for the purpose of the spectrometer validation⁴.

☞ 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.
<p>Source performance has decreased significantly because the end of its service lifetime is nearly reached.</p> <ul style="list-style-type: none"> ➤ This problem is indicated by the following message <i>End of average lifetime is nearly reached, spare part will be required.</i> ➤ Note: To find out of which component - either laser or source - the end of the average lifetime is nearly reached, open in OPUS the <i>Instrument Status</i> dialog window. The component in question has the status WARNING. 	<p>Order a replacement source. For the order number refer to section B.1. After receiving the replacement source, replace the defective source.</p> <p>☞ For information about the proper installation and the replacement procedure, see the document <i>INVENIO - Source Replacement Instructions</i> which is added to the replacement source.</p> <hr/> <p>i Replacing the source is a recommended Bruker service delivery.</p> <hr/> <p>☞ For the Bruker service contact data, see section 1.6.</p>
<p>Sample compartment windows are dirty or their IR light transparency has declined significantly in the course of time.</p> <p>Note: Especially hygroscopic materials tend to become IR-non-transparent if exposed to humidity.</p>	Order replacement windows. For the order number, see section B.3. After receiving them, replace them as described in section 5.12.

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 for the purpose of extending the spectral range.)
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
<p>The optical material of the beamsplitter is dirty or has become IR-non-transparent or the beamsplitter is damaged.</p> <p>Note: Especially hygroscopic materials tend to become IR-non-transparent if exposed to humidity.</p>	<p>Order a replacement beamsplitter. For the order number refer to section B.2. After receiving it, replace the beamsplitter as described in section 5.10.</p>
<p>The spectral ranges of optical components (source, beamsplitter and detector) which you have selected in OPUS are different.</p> <p>The spectral range of the sample compartment windows does not match with the spectral range of the selected optical components (source, beamsplitter and detector).</p>	<p>Select source, beamsplitter and detector of a matching spectral range and repeat the OVP test.</p> <p>Exchange the sample compartment windows as described in section 5.12. Afterwards, repeat the OVP test.</p> <ul style="list-style-type: none"> ☞ The optical components of the available spectral range packages are listed in section 2.2. ☞ For information about the spectral range of the available sources, detectors, beamsplitters and sample compartment windows refer section 4.5.2, 4.5.3, 4.5.4 and 4.5.5.)
<p>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.</p>	<p>After having filled in liquid nitrogen, wait about 20 minutes. Then, repeat the OVP test.</p>
<p>Ice formation on the MCT detector dewar.</p> <ul style="list-style-type: none"> ➤ This problem becomes apparent by a failed ice band test. This test is part of the PQ test procedure. 	<p>Evacuate the MCT detector dewar as described in section 6.3. Afterwards, repeat the OVP test.</p>
<p>Air humidity content inside the spectrometer is too high.</p> <ul style="list-style-type: none"> ➤ Note: This problem becomes apparent by a failed water vapor test. This test is part of the OQ test procedure. 	<p>Reduce the air humidity content inside the spectrometer by purging the spectrometer with dry air or nitrogen gas. Afterwards, repeat the OVP test.</p> <ul style="list-style-type: none"> ☞ For information about purging the spectrometer, see section 5.8.
<p>Interferogram peak position has shifted.</p>	<p>Save the new peak position using the OPUS software as described in section 5.13.3. Afterwards, repeat the OVP test.</p>
<p>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.) ...</p>	<p>... contact the Bruker service.</p> <ul style="list-style-type: none"> ☞ 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.	<p>The data cable type (cross-over or straight), which has to be used, depends on the realized connection variant.</p> <p>☞ For information about which data cable type has to be used for which connection variant, see section 3.8.1.</p> <p>Procure a data cable of the correct type. and replace the data cable.</p>
Data cable connector is loose.	<p>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.</p> <p>☞ See section 3.8.1.</p>
Data cable is damaged.	<p>Check the data cable for damages. If it shows signs of damages, replace it.</p>
Spectrometer does not start up.	<p>Check whether the spectrometer is connected to a mains socket outlet.</p> <p>☞ See section 3.6.</p> <p>Check whether the mains supply meets the requirements.</p> <p>☞ See section 3.5.</p> <p>Check whether the spectrometer is switched on. If not, do so now.</p> <p>☞ See section 5.2.</p> <p>If these actions do not solve the problem contact the Bruker service.</p> <p>☞ For the contact data, see section 1.6.</p>
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.)	<p>Assign the correct IP address to the spectrometer.</p> <p>☞ See section 3.8.6.</p>
TCP/IP settings mismatch between spectrometer and computer/network.	<p>☞ Refer to the documentation of the operating system Windows.</p>

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 *ipconfig/all* and press the ENTER key again.
6. Take a screenshot of the dialog (fig. 7.10) and provide it for your network administrator.

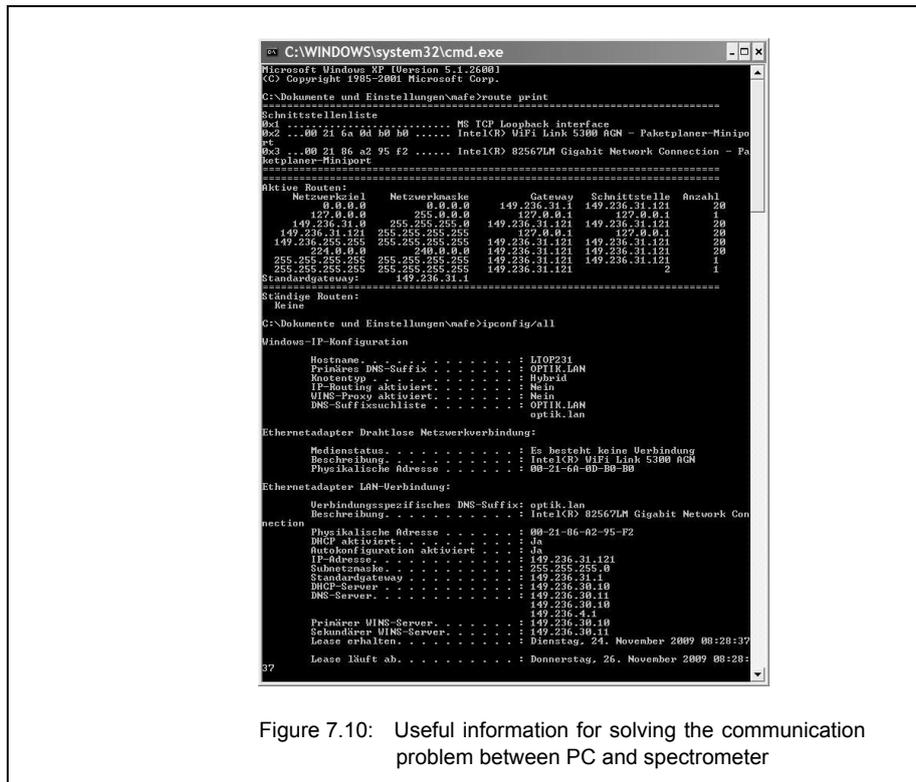


Figure 7.10: Useful information for solving the communication problem between PC and spectrometer

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 panel PC and touch screen: 32 cm height with panel PC and touch screen: 50 cm height with open, large-sized sample compartment: 62 cm
Spectral range	standard: With the standard optical components (KBr beamsplitter, DLaTGS detector and MIR source) the following spectral range is achieved: MIR: 8,000 to 350 cm^{-1} optional: With the corresponding optional optical components, the following spectral ranges can be achieved: Far IR: 680 to 15 cm^{-1} Near IR: 15,500 to 4,000 cm^{-1} Visible/UV: 28,000 to 9,000 cm^{-1}
Spectral resolution	better than 0.16 cm^{-1}
Wavenumber accuracy	better than 0.005 cm^{-1} @ 1,554 cm^{-1}
Photometric accuracy	better than 0.1% T
Scan speed	standard: 8 velocities from 1.6 to 80 kHz (1.0 to 50 mm/sec opd) optional: 12 velocities from 1.6 to 160 kHz (1.0 to 100 mm/sec opd)
Source	standard: MIR source (globar, electronically stabilized, air-cooled) optional: various sources for measurements in the NIR, MIR, FIR, UV and VIS region (See also section 4.5.2.)
Beamsplitter	standard: KBr beamsplitter optional: various beamsplitters for measurements in the NIR, MIR, FIR, UV and VIS region (See also section 4.5.4.)
Detector	standard: High sensitivity DTGS detector with KBr window optional: various detectors for measurements in the NIR, MIR, FIR, UV and VIS region (See also section 4.5.3.)

Parameter	Specification
Sample compartment window	standard: KBr window optional: various window materials for measurements in the NIR, MIR, FIR, UV and VIS region (See also section 4.5.5.)
Laser	INVENIO R is a laser class 1 product containing a laser class 2 laser according to EN 60825-1:2007. The laser emits red light with a wavelength of 633 nm. The rated power output is 0.8 mW.
Interferometer	ROCKSOLID permanently aligned, wear-free and high stability interferometer
Sample compartment (large-sized)	Dimensions: 25.5cm (W) x 27.0cm (D) x 22.5 cm (H) The purgeable sample compartment is separated from the optical bench by windows or automatic shutters.
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, TCP/IP protocol

A.2 Power supply

Parameter	Specification
Voltage (input range)	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
Q 328/I7	MIR source, mounted, 12 V
Q 428/I7	NIR source, mounted, 12 V
Q 101/B	HeNe laser module
S 119/B	Desiccant cartridge (regenerable desiccant), package containing 2 cartridges

B.2 Beamsplitter

Order number	Replacement part
T303/IR	KBr beamsplitter, standard, (MIR), 8,000 to 350 cm^{-1}
T304/IR	KBr beamsplitter, broad band, (MIR), 10,000 to 380 cm^{-1}
T401/IR	CaF_2 beamsplitter (NIR), 15,000 to 1.200 cm^{-1}
T502/IR	Quartz beamsplitter (VIS) 30,000 to 3,500 cm^{-1}
T222/IR	Multilayer beamsplitter (FIR), 680 to 30 cm^{-1}
T204/IR	Mylar beamsplitter, 25 μm (FIR), 120 to 30 cm^{-1}
T205/IR	Mylar beamsplitter, 50 μm (FIR), 55 to 10 cm^{-1}
T410/IR	Alignment beamsplitter (glass)
T230/IR	Solid state beamsplitter based on silicon plate, (FIR) 600 to 30 cm^{-1} Note: In conjunction with the FIR source (Hg-arc), the spectral range is extended to 10 cm^{-1} .
T240/IR	Wide range beamsplitter (MIR and FIR), 6,000 to 10 cm^{-1} suitable for spectral resolution up to 0.4 cm^{-1}
T240-T/IR	Wide range beamsplitter (thin, MIR and FIR), 6,000 to 10 cm^{-1} suitable for spectral resolution up to 0.9 cm^{-1}

B.3 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-I1	Quartz window (45 x 2 mm)
F162-I11	ZnSe window (wedge 6 mrad, 45 x 3 mm)
F162-I17	BaF ₂ window (wedge, 45 x 3 mm)
F162-I3	CaF ₂ window (wedge 6 mrad, 45 x 3 mm)
F162-I4	NaCl window (wedge 6 mrad, 45 x 3 mm, protected)
F162-I5	KBr window (wedge 6 mrad, 45 x 3 mm)
F162-I6	KRS-5 window (wedge 6 mrad, 45 x 3 mm)
F162-I7	CsI window (45 x 3 mm, protected)
F162-I9	Polyethylene window (45 x 3 mm)

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 R, 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.

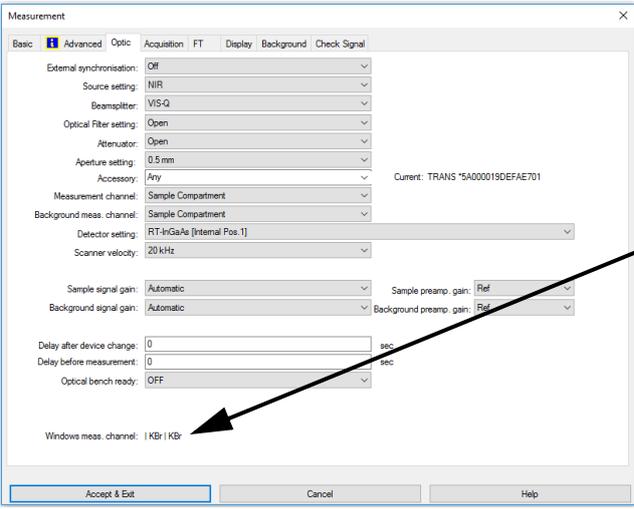
Advanced parameters	Settings and values
Resolution	4
Sample/Background Scan Time	6 scans
Save Data	from 7500 to 400cm ⁻¹
Result Spectrum	Transmittance
Data Blocks to be saved	Transmittance, Single Channel and background
Optics Parameter	Settings
Source Setting	MIR
Beam splitter	KBr
Optical Filter Setting ^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 perforated grid wheel with different grid 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 8mm. 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:



Measurement

Basic **Advanced** Optic Acquisition FT Display Background Check Signal

External synchronisation: OFF

Source setting: NIR

Beamsplitter: VIS-Q

Optical Filter setting: Open

Attenuator: Open

Aperture setting: 0.5 mm

Accessory: Any

Measurement channel: Sample Compartment

Background meas. channel: Sample Compartment

Detector setting: RT-InGaAs [Internal Pos.1]

Scanner velocity: 20 kHz

Sample signal gain: Automatic

Background signal gain: Automatic

Delay after device change: 0 sec

Delay before measurement: 0 sec

Optical bench ready: OFF

Windows meas. channel: 1 KBr | KBr

Accept & Exit Cancel Help

Current: TRANS *SA000019DEFAE701

Sample preamp. gain: Ref

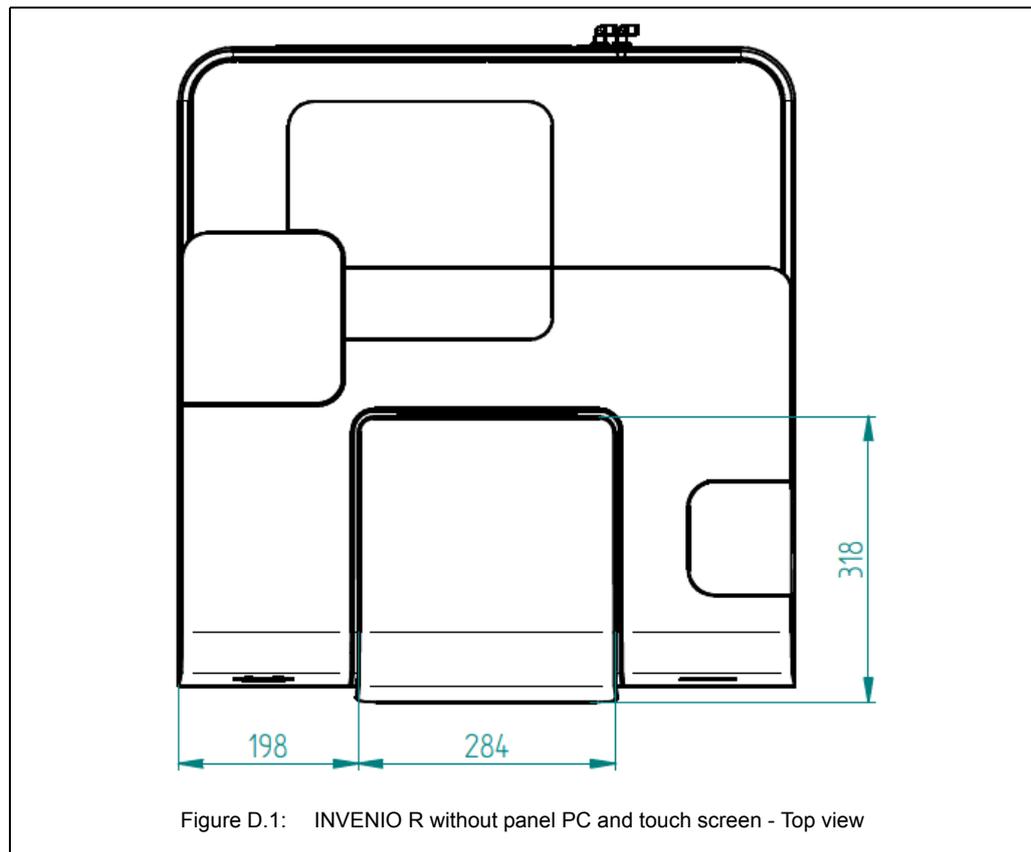
Background preamp. gain: Ref

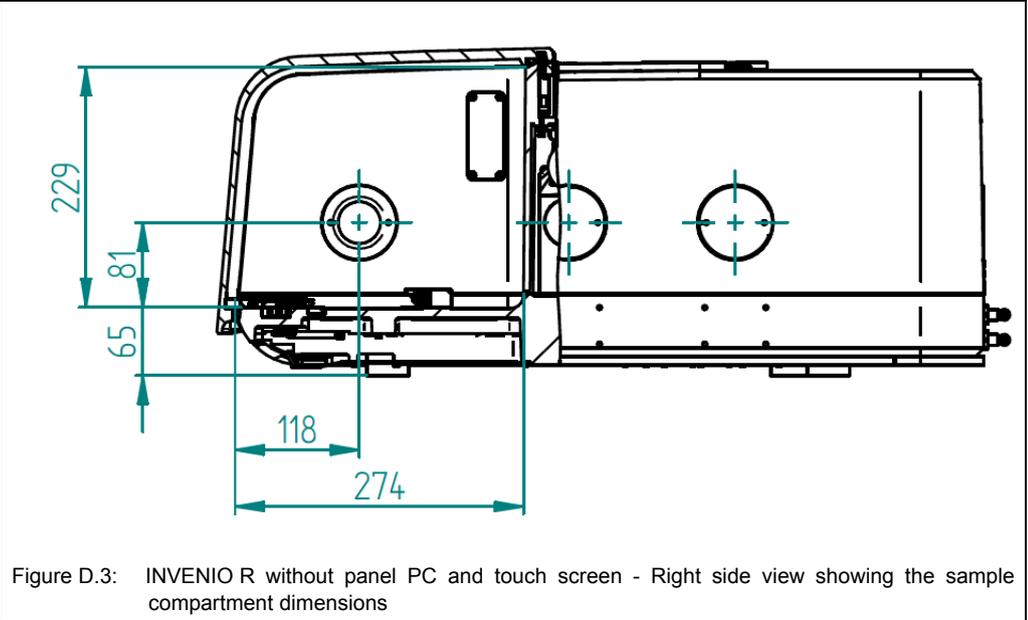
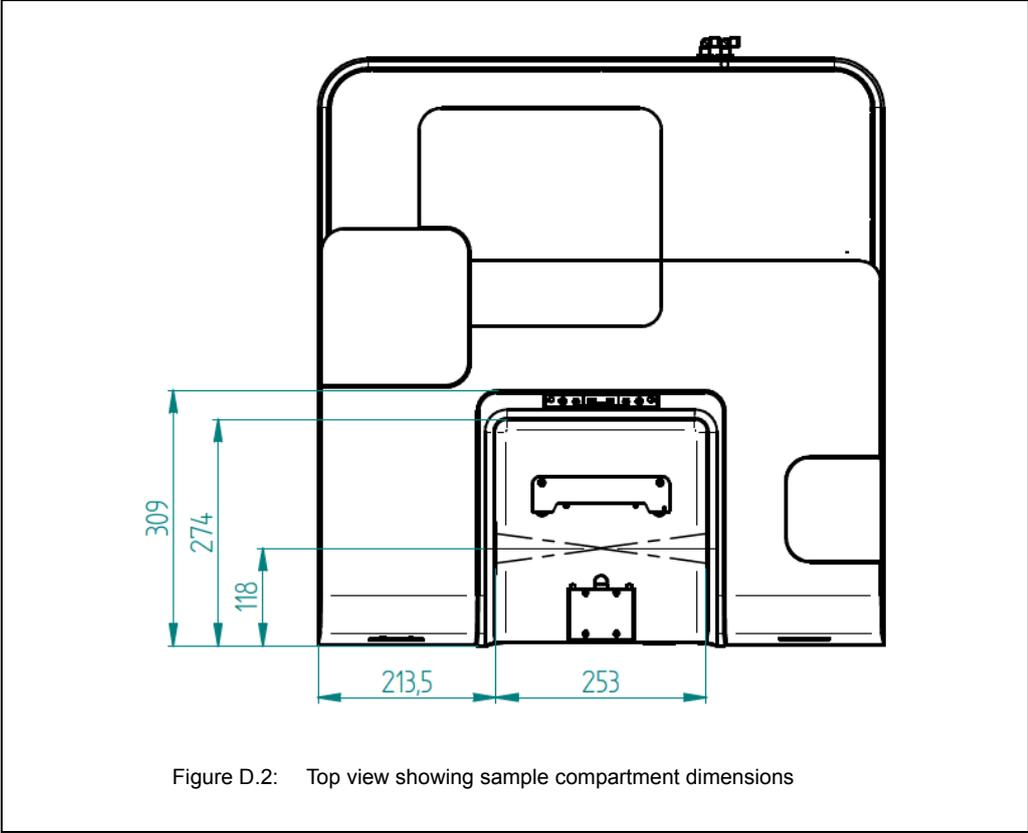
Display of the installed windows
 Note: The order in which the windows are displayed in OPUS corresponds with the optical beam path starting from the IR source to the detector.
 For information about the optical beam path, see section 4.6.

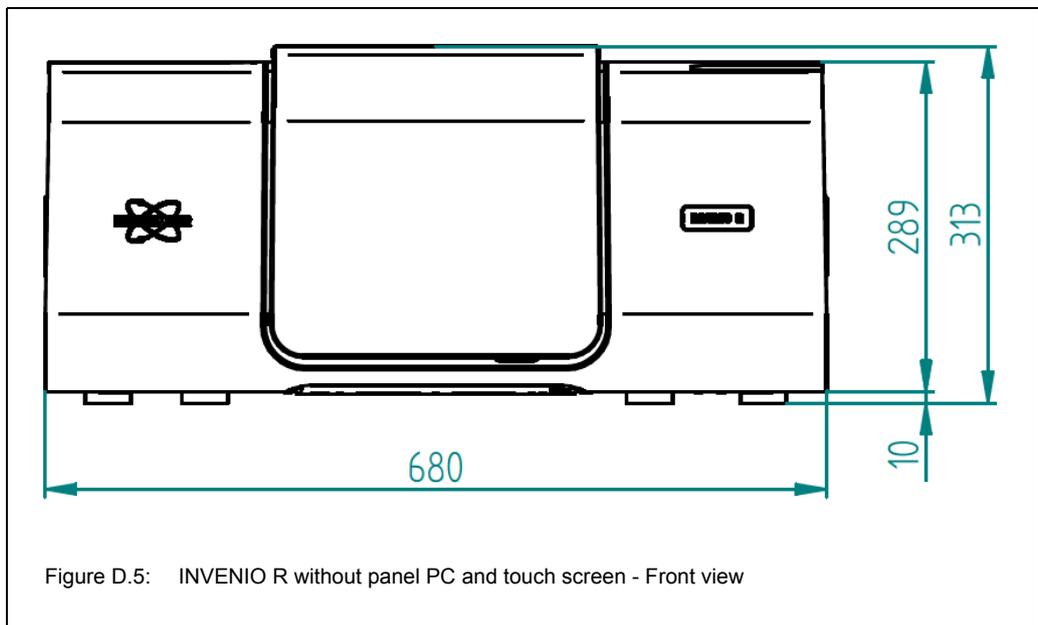
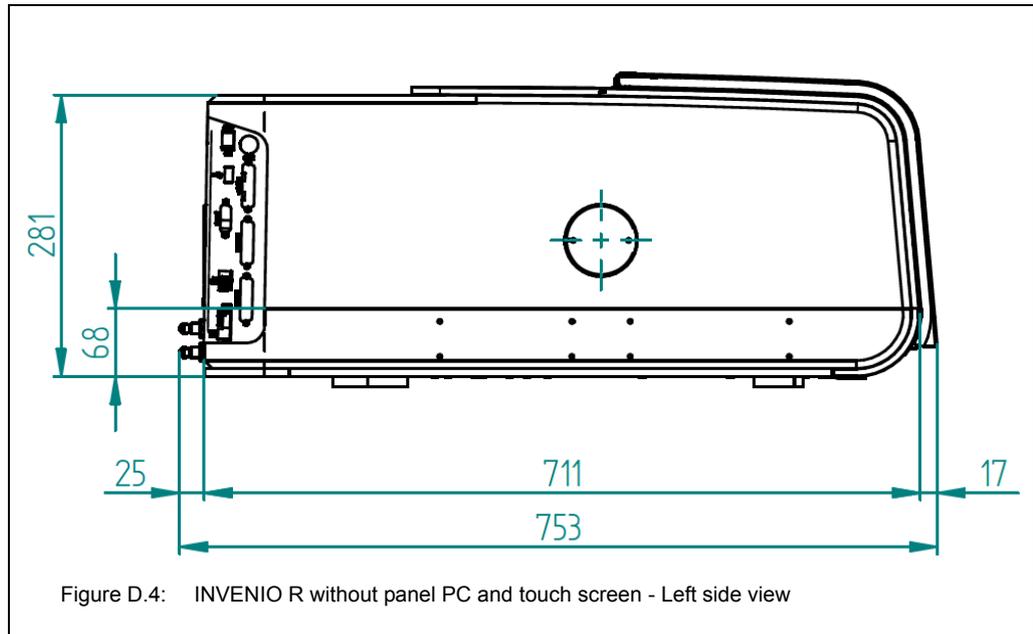
Figure C.1: OPUS Measurement dialog - Optics page

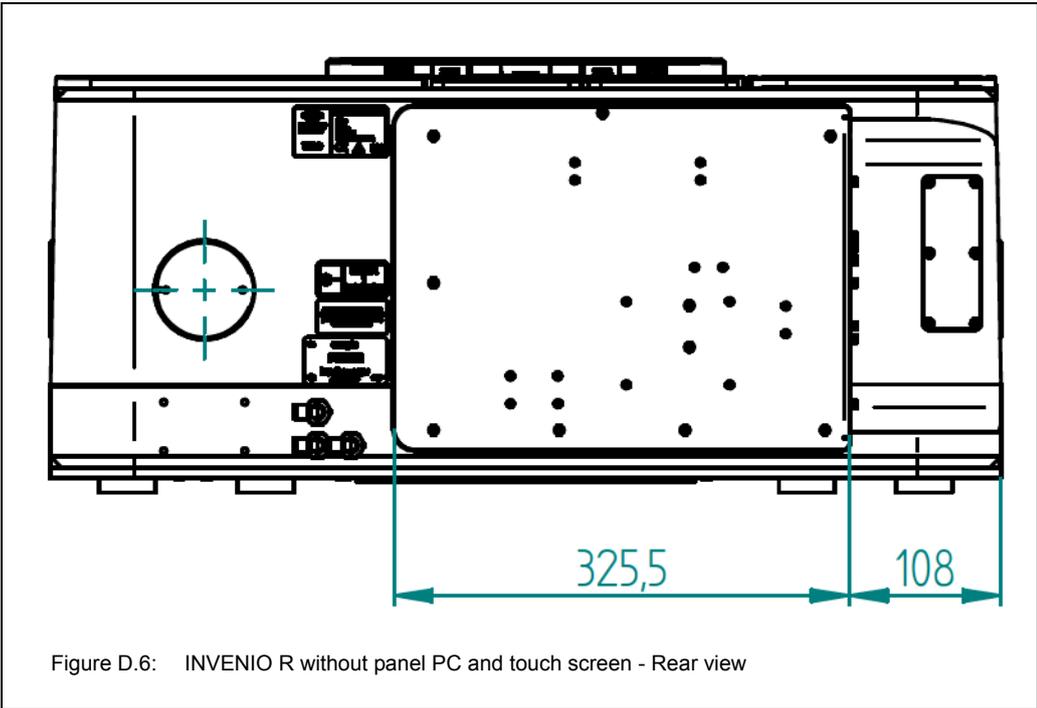
D Dimensional drawings

D.1 INVENIO R without panel PC and touch screen

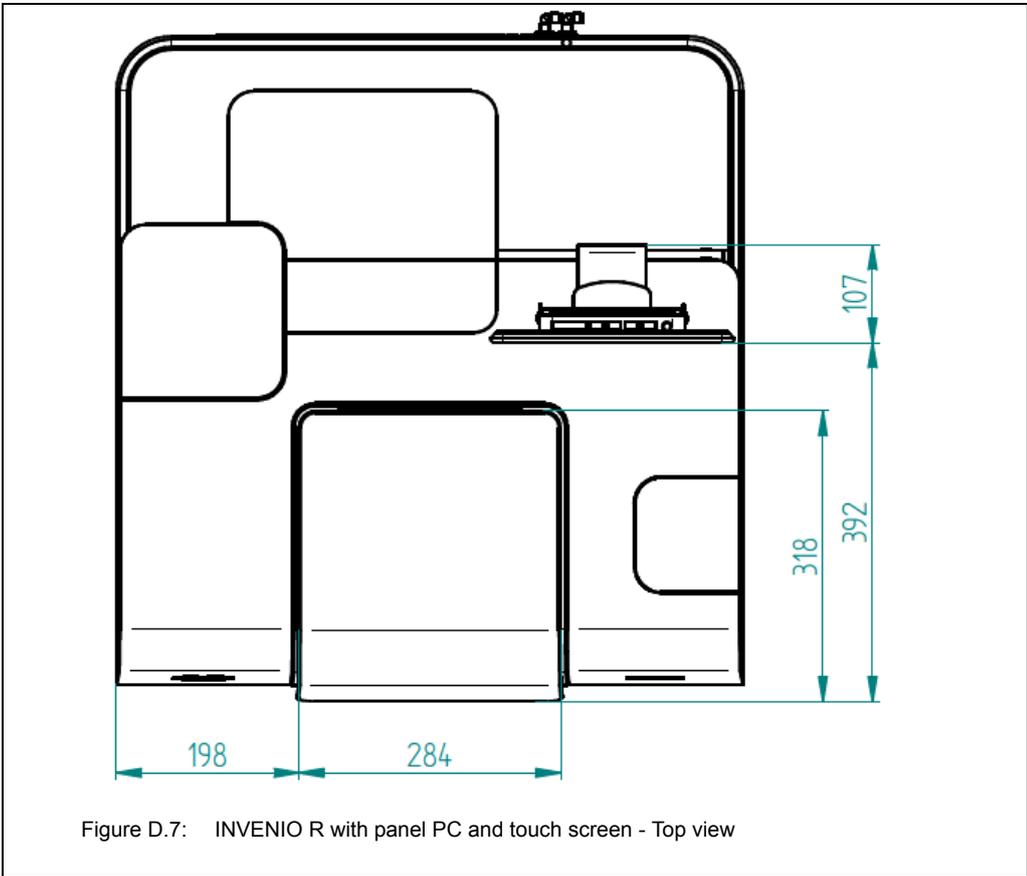


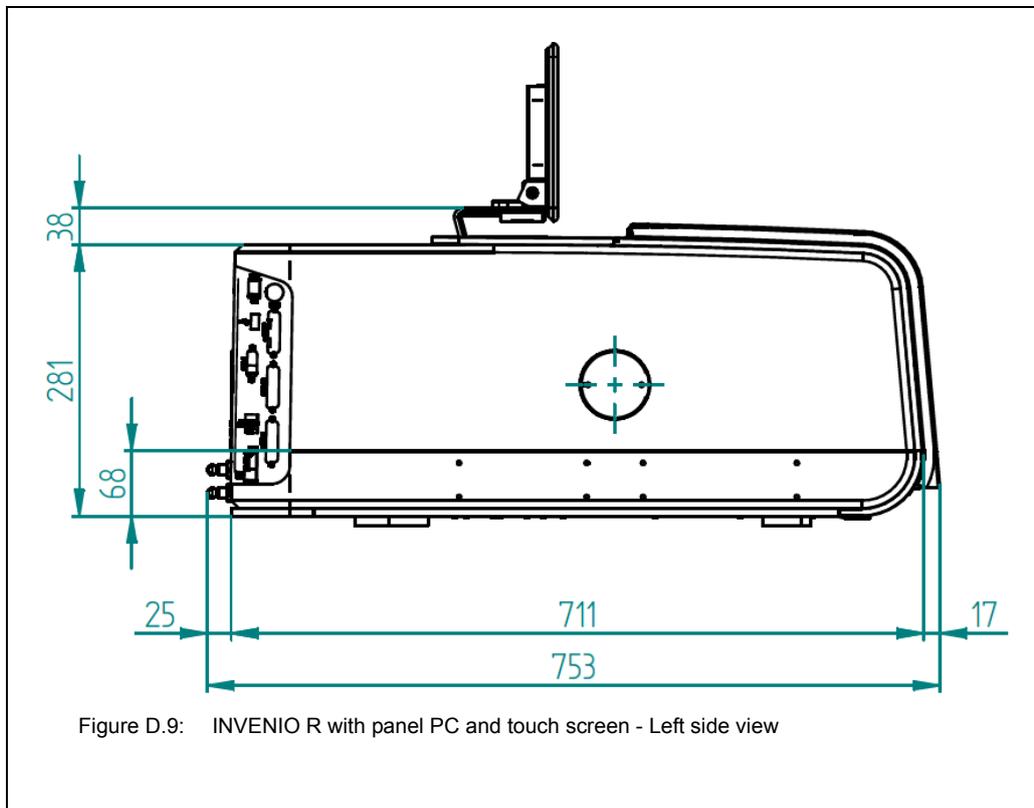
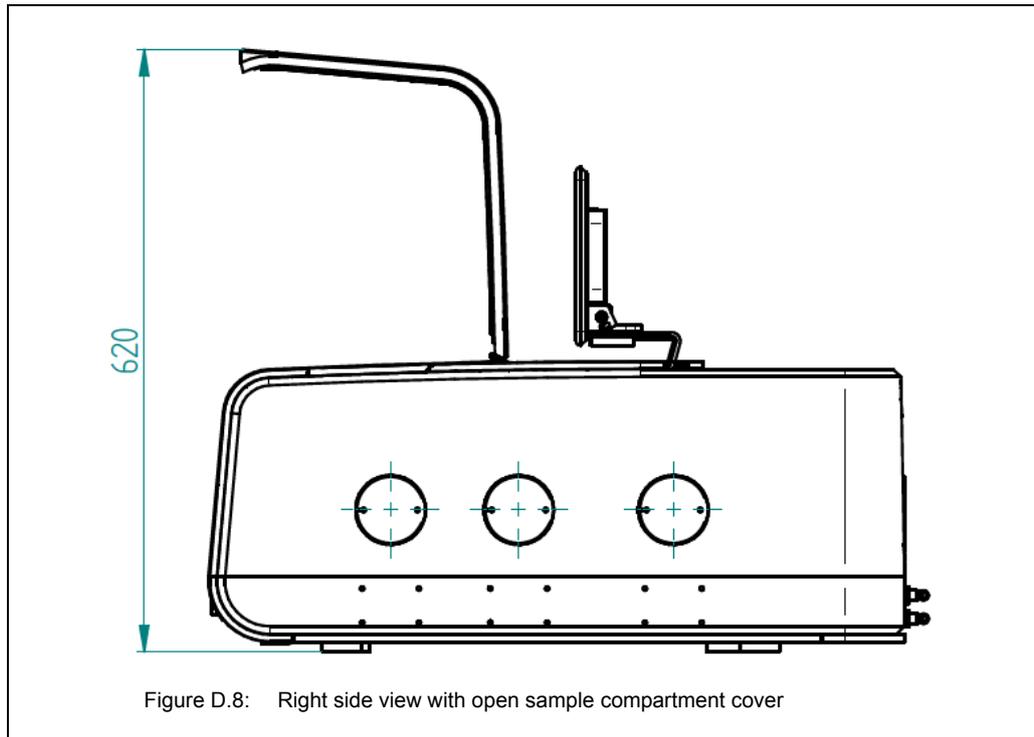


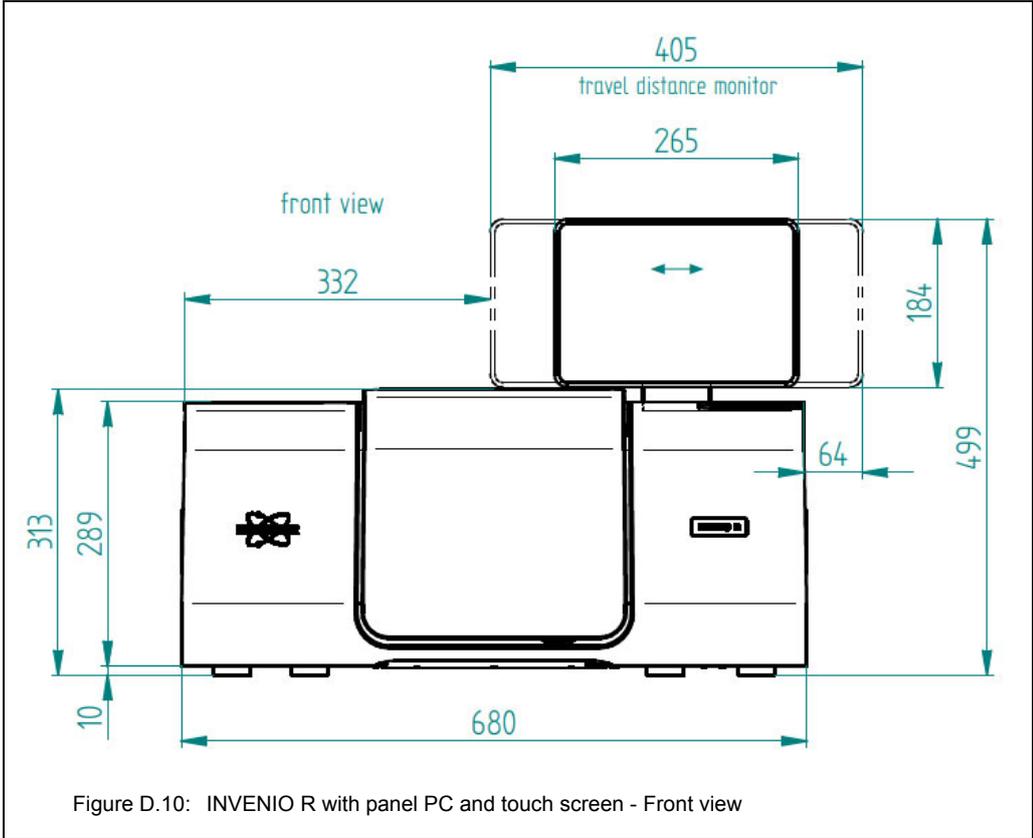




D.2 INVENIO R with panel PC and touch screen







E Spectrometer firmware

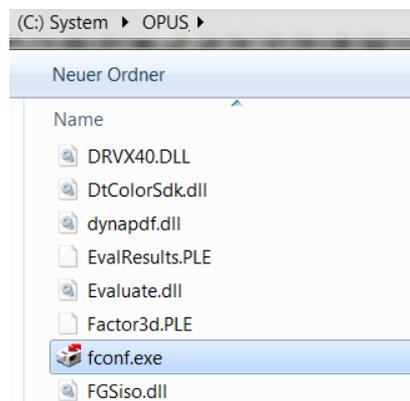
E.1 General information

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.)

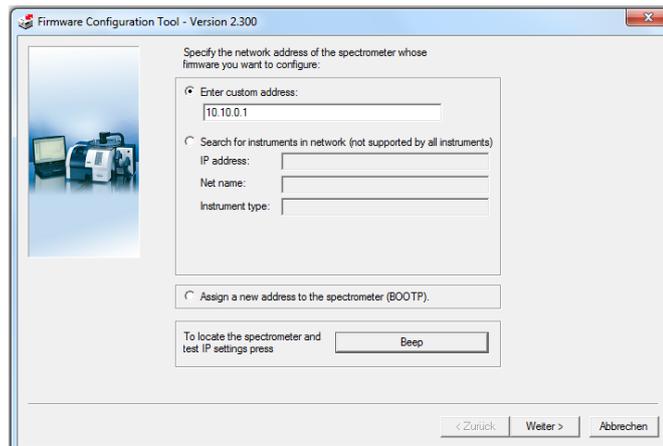
E.2 Starting the FCONF program

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



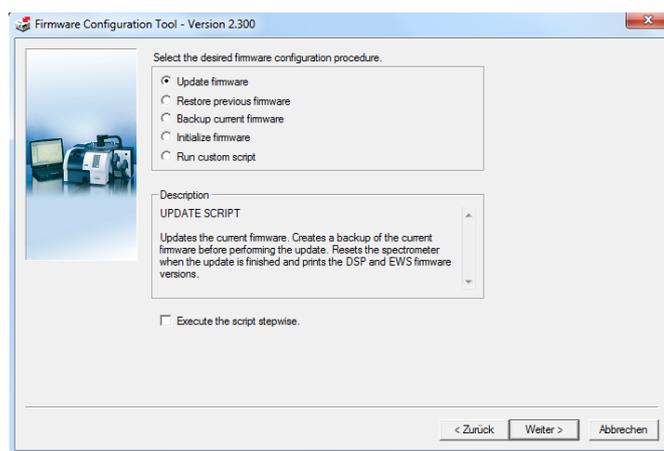
-  Note: In case of updating the spectrometer firmware, the firmware update is typically delivered on CD or by e-mail. If the firmware update has been delivered on a CD, start the FCONF program directly from the CD by double-clicking on the `fconf.exe` file and proceed as described below. If the firmware 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:



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



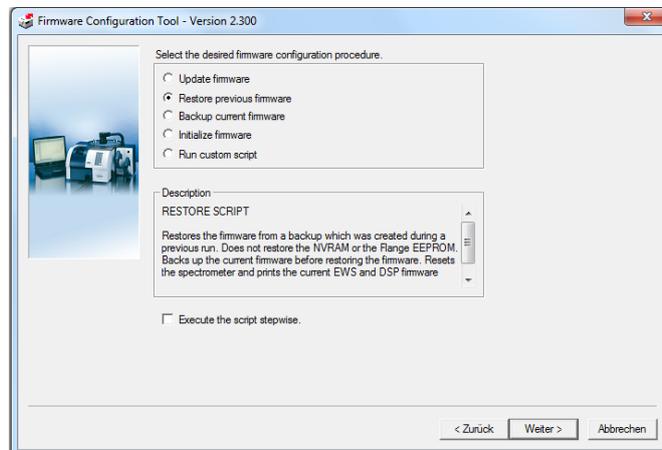
1. Activate the *Update firmware* option button.
2. Click on the *Next* button.
3. Select the directory (run folder) in which the backup data are to be stored.
 Note: It is recommended to accept the displayed default directory.
4. Follow the next on-screen instructions.

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.

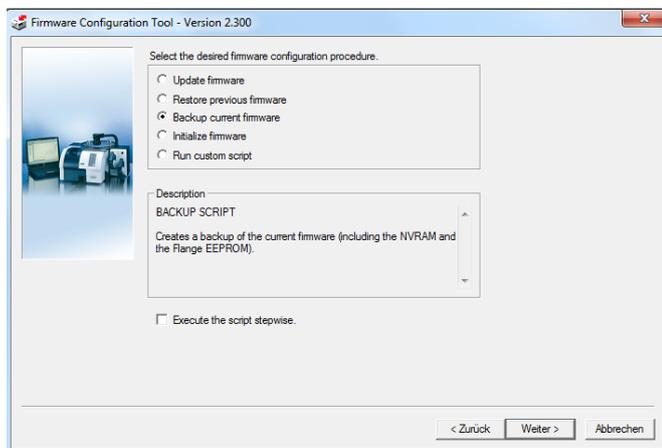


1. Activate the *Restore previous firmware* option button.
2. Click on the *Next* button.
3. Select the directory (run folder) which contains the firmware version you intend to restore.
4. Follow the next on-screen instructions.

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

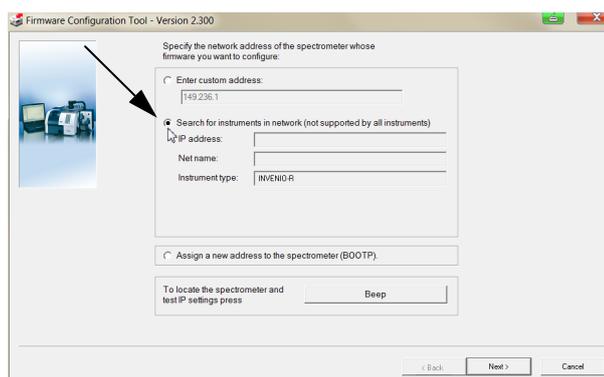


1. Activate the *Backup current firmware* option button.
2. Click on the *Next* button.
3. Follow the on-screen instructions.

E.6 Retrieving the spectrometer IP address

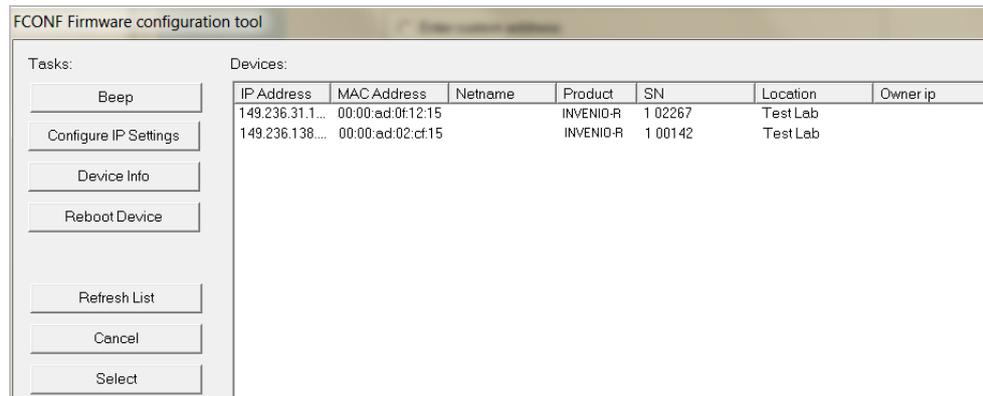
In case you need to know the currently assigned IP address of the spectrometer, you can retrieve it by proceeding as follows:

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



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:



The screenshot shows the 'FCONF Firmware configuration tool' window. On the left, there is a 'Tasks:' panel with buttons for 'Beep', 'Configure IP Settings', 'Device Info', 'Reboot Device', 'Refresh List', 'Cancel', and 'Select'. On the right, there is a 'Devices:' table with the following data:

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

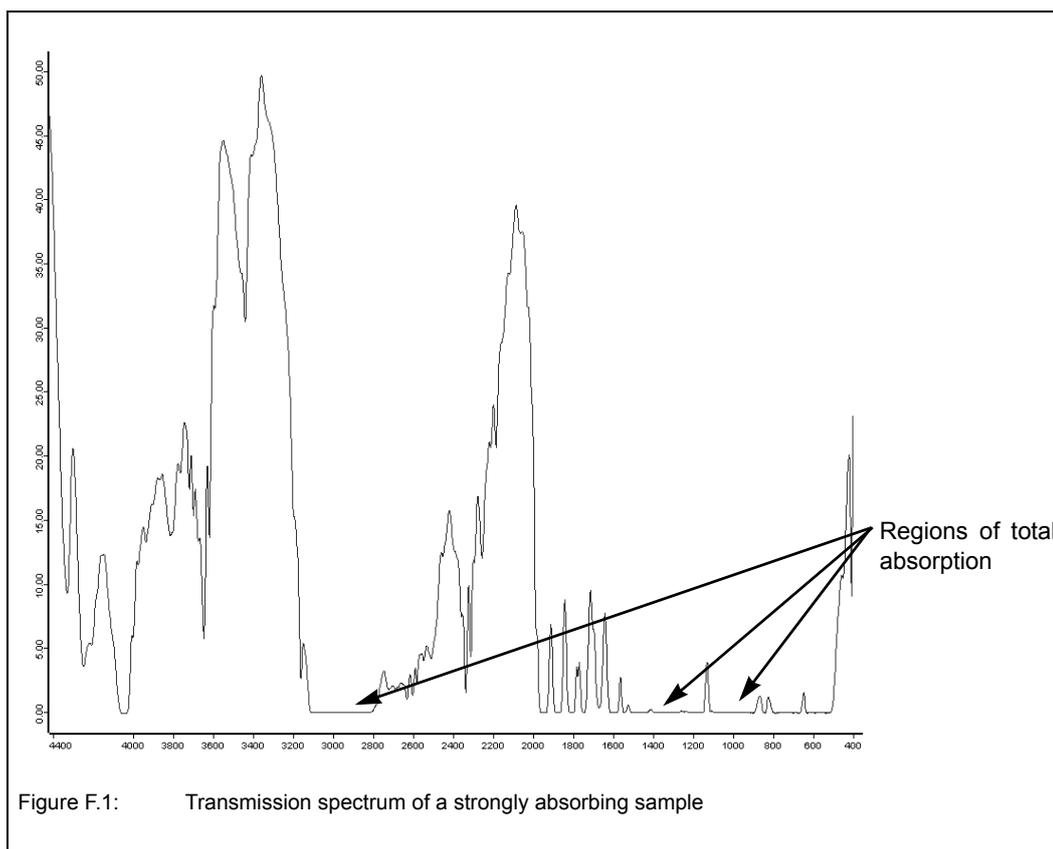
According to Lambert Beer's Law, the absorbance (i.e. peak intensity) in an absorbance spectrum is directly proportional to the component concentration in the sample, path-length of the sample and the absorptivity.

$$A = \epsilon bC$$

Symbol	Description	Typical measuring units
A	Absorbance at a given wavelength	None
ϵ	Molar absorptivity (a proportionality constant)	$l \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$
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.



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 literature¹.) 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.

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 plates¹
 - Preparing a sample solution
 - Preparing a Nujol mull²
 - 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 FT-IR 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 a 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 disulfide, 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 1375 cm^{-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 1330 cm^{-1} , Fluorolube above 1330 cm^{-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 vase-line-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 pure 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 $3,480\text{cm}^{-1}$ and $1,950$ to $1,300\text{cm}^{-1}$ and below 500cm^{-1}) and in some 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 too 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 CaF₂) 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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