

minispec

minispec mq-one SeriesUser ManualVersion 004

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1 About This Manual

This manual provides instructions for the following mq-one models:

- mg-one SFC Analyzer
- · mq-one Spin Finish Analyzer
- · mq-one Fat Analyzer
- mq-one Hydrogen Analyzer
- · mq-one Polymer Analyzer
- · mq-one Seed Analyzer
- · mq-one Seed XL Analyzer

This manual enables safe and efficient handling of the device.

This manual is an integral part of the device, and must be kept in close proximity to the device where it is permanently accessible to personnel. In addition, instructions concerning labor protection laws, operator regulations tools and supplies must be available and adhered to.

Before starting any work, personnel must read the manual thoroughly and understand its contents. Compliance with all specified safety and operating instructions, as well as local work safety regulations, are vital to ensure safe operation.

The figures shown in this manual are designed to be general and informative and may not represent the specific Bruker model, component or software/firmware version you are working with. Options and accessories may or may not be illustrated in each figure.

1.1 Policy Statement

It is the policy of Bruker to improve products as new techniques and components become available. Bruker reserves the right to change specifications at any time.

Every effort has been made to avoid errors in text and figure presentation in this publication. In order to produce useful and appropriate documentation, we welcome your comments on this publication. Support engineers are advised to regularly check with Bruker for updated information.

Bruker is committed to providing customers with inventive, high quality products and services that are environmentally sound.

1.2 Symbols and Conventions

Safety instructions in this manual are marked with symbols. The safety instructions are introduced using indicative words which express the extent of the hazard.

In order to avoid accidents, personal injury or damage to property, always observe safety instructions and proceed with care.





DANGER indicates a hazardous situation which, if not avoided, will result in death or serious injury.

This is the consequence of not following the warning.

- 1. This is the safety condition.
- ▶ This is the safety instruction.

MARNING



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

This is the consequence of not following the warning.

- 1. This is the safety condition.
- ► This is the safety instruction.

A CAUTION



CAUTION indicates a hazardous situation, which, if not avoided, may result in minor or moderate injury.

This is the consequence of not following the warning.

- 1. This is the safety condition.
- ► This is the safety instruction.

NOTICE

NOTICE indicates a property damage message.

This is the consequence of not following the notice.

- 1. This is a safety condition.
- ► This is a safety instruction.

SAFETY INSTRUCTIONS

SAFETY INSTRUCTIONS are used for control flow and shutdowns in the event of an error or emergency.

This is the consequence of not following the safety instructions.

- 1. This is a safety condition.
- ► This is a safety instruction.



This symbol highlights useful tips and recommendations as well as information designed to ensure efficient and smooth operation.

1.3 Font and Format Conventions

| Type of Information | Font | Examples |
|--|---|--|
| Shell Command, Commands, "All what you can enter" | Arial bold | Type or enter fromjdx zg |
| Button, Tab, Pane and Menu Names "All what you can click" | Arial bold, initial letters capitalized | Use the Export To File button. Click OK. Click Processing |
| Windows, Dialog Windows, Pop-up Windows Names | Arial, initial letters capitalized | The Stacked Plot Edit dialog will be displayed. |
| Path, File, Dataset and Experiment Names Data Path Variables Table Column Names Field Names (within Dialog Windows) | Arial Italics | \$tshome/exp/stan/nmr/ lists expno, procno, |
| Parameters | Arial in Capital Letters | VCLIST |
| Program Code Pulse and AU Program Names Macros Functions Arguments Variables | Courier | go=2 au_zgte edmac CalcExpTime() XAU(prog, arg) disk2, user2 |
| AU Macro | Courier in Capital Letters | REX PNO |

Table 1.1: Font and Format Conventions

About This Manual

2 Safety

This manual contains notices which should be observed to ensure your own personal safety as well as to protect the spectrometer and the connected equipment.

2.1 Intended Use

The minispec mq-one is a pulsed time-domain NMR analyzer used for the monitoring of the hydrogen nuclei.

This product is intended to be used solely for measurements on industrial samples. The minispec mq-one has not been tested for compliance with regulatory agencies for human subject exposure to radio frequency irradiation. Although no indication that any danger exists, under no circumstance is this product intended for measurements on humans.

2.2 Qualified Personnel

The minispec mq-one may only be set up and operated in conjunction with the instructions in this manual. Only qualified personnel should be allowed to work on this equipment. The primary installation, maintenance and repair of the minispec mq-one may only be carried out by personnel which are authorized by BRUKER.

All repairs, adjustments and alignments performed on any components of the minispec must be carried out strictly in accordance with the established safety practices and standards of the country where the instrument is installed.

2.3 Correct Usage

This device and its components may only be used in the way discussed with a BRUKER specialist and in connection with devices or components from other manufacturers which have been approved or recommended by BRUKER.



Note: This product can only function correctly and safely if it is transported, stored, set up and installed correctly, and operated and maintained as recommended by BRUKER.

2.4 Electrical Safety

There is no danger of electrical shock during routine operation of the spectrometer, however the following precautions must be followed to assure user safety and protection of the instrument.

MARNING

Electrical hazard from electrical shock





- ▶ Place the mains power switch in the OFF position (direction labeled "0" on the switch).
- ▶ Disconnect the device from the electrical power supply before maintenance. Use a voltmeter to verify that the device is not under power!
- ▶ Be sure that the power supply cannot be reconnected without notice.
- ► Ensure that all warning labels are in place.
- ▶ Only trained personnel should carry out maintenance.



The safety precautions applicable to any electronic device connected to AC power must be observed.

Always use the power cable that is delivered with the product.

If replacement of the power cable is necessary, make sure that the ratings with regard to the power consumption of the device are suitable.

⚠ WARNING

Electrical hazard from stored electrical charge

A life threatening shock or material damage may result from a stored electrical charge. Never touch electrical contacts or semiconductor chips with any object (conductive or nonconductive) unless all of the following conditions are met:



- ► The power switch is off.
- ▶ The power plug is disconnected from either the power socket or the main power socket on the spectrometer.
- ▶ The conductive object and you are grounded.
- ⇒ This precaution prevents the possibility of electrical shock from stored charge within the power supply circuitry or the transfer of static charge that can damage semiconductor chips.



Note: No other components within the spectrometer should be touched (even with the power off) without first contacting a Bruker service representative to obtain all necessary instructions, to ensure user and spectrometer safety.

2.5 Lifting Safety

The standard magnet unit may weigh up to 150 kg depending on the type of the mq-one Analyzer, to ensure safety the follow safety instructions must be followed:

A CAUTION

Risk of injury from lifting heavy objects.



The unit is very heavy and may lead to injury when lifting.

- ▶ Do not attempt to lift the unit over the edge of the carton, remove the carton first.
- ▶ Do not attempt to lift the unit on your own or without necessary precaution against injury.
- ► Use a hoist if available.
- ▶ Follow the step-by-step instructions in the installation section of this manual.

2.6 Personal Safety

2.6.1 Safety for Persons Wearing Pacemakers

The instrument contains strong magnetic fields, some of which extend beyond the magnet unit house (see stray field diagram below). These pose no danger to routine users, but are hazardous to persons with heart pacemakers or other medical implantations.

WARNING

Risk to life due to high magnetic fields

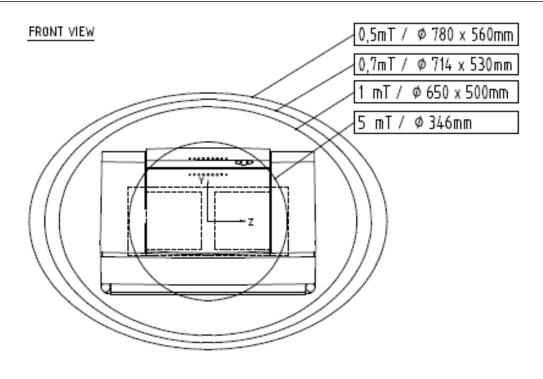
A magnetic field of more than 0.5 mT (5 Gauss) is life-threatening for people with pacemakers or active metal implants. Exposure to more than 8 T can cause damage to health. Duration of exposure (8 h/day) above the limit of 200 mT can cause damage to health. Ferromagnetic tools in the magnetic field are significantly hazardous. Disks and electronic devices may be damaged.

▶ Mark the magnetic field of more than 0.5 mT (5 Gauss) before start up.



- ► Keep people with active medical implants or heart pacemakers away from the 0.5 mT (5 Gauss) area.
- ▶ The permanent workplace of employees must be outside the 0.5 mT (5 Gauss) area.
- ▶ Do not stay or work at magnetic fields of more than 8 T.
- ▶ Prevent exposure of more than 200 mT for more than 8 h/day.
- ▶ Keep disks, credit cards and electronic devices away from the identified area.
- ▶ Do not use ferromagnetic tools or items within the identified area.
- Only use non-ferromagnetic transportation dewars or pressure cylinders for the cryogenic agents.
- ▶ Only use non-ferromagnetic ladders or steps.
- ▶ Remove magnetic items (jewelry, watches, pens etc.) before carrying out maintenance work.

2.6.1.1 Stray Field Plot 0.47T/Air Gap 25 mm



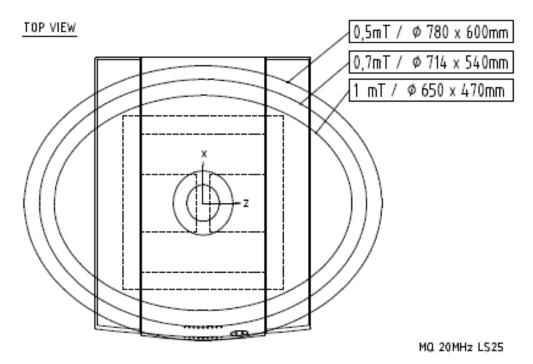
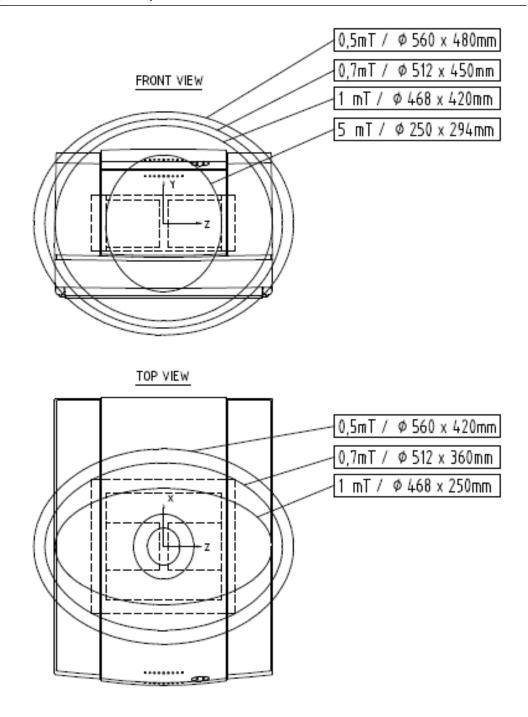


Figure 2.1: Example of a Stray Field Plot for a Typical 0.47T / 20 MHz Magnet / Air Gap 25 mm

The above stray field plot applies to the following mq-one systems:

- mq-one Polymer Analyzer
- mq-one Fat Analyzer
- mq-one Hydrogen Analyzer
- mq-one Spin Finish Analyzer

2.6.1.2 Stray Field Plot 0.47T/Air Gap 20 mm



MQ 20MHz LS20

Figure 2.2: Example of a Stray Field Plot for a Typical 0.47T / 20 MHz Magnet / Air gap 20 mm

The above stray field plot applies to the following mq-one systems:

• mq-one SFC Analyzer

2.6.1.3 Stray Field Plot 0.23T

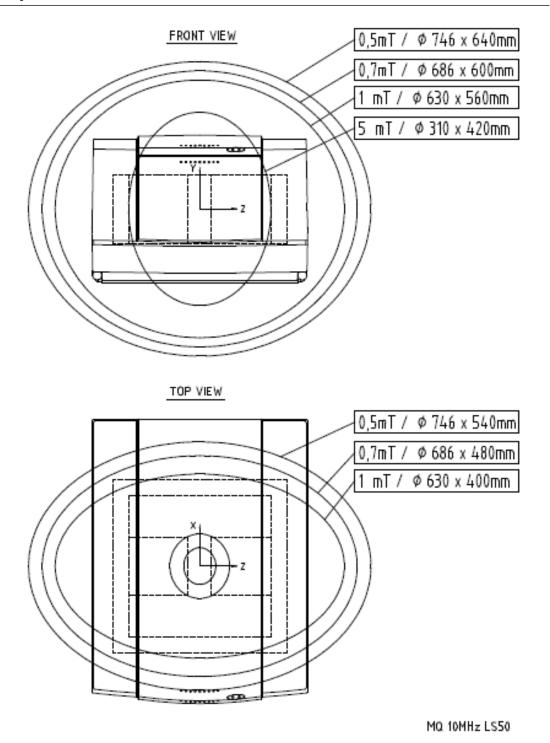


Figure 2.3: Example of a Stray Field Plot for a Typical 0.23T / 10 MHz Magnet

The above stray field plot applies to the following mq-one systems:

• mq-one Seed Analyzer

2.6.1.4 Stray Field Plot 0.17T

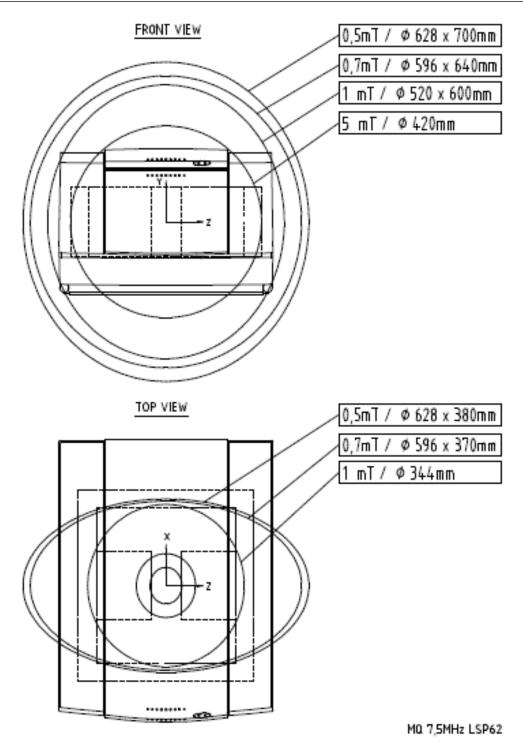


Figure 2.4: Example of a Stray Field Plot for a Typical 0.17T / 7.5 MHz Magnet

The above stray field plot applies to the following mq-one systems:

• mq-one Seed XL Analyzer

2.6.2 Safety When Working with VT Probe Systems (mq-one Polymer only)

WARNING



Danger of injury due to burns (hot/cold) when working with VT probe systems

The operator may burn their hands or fingers when touching a very hot or cold sample, or the top of the VT probe.

- ▶ Wear protective gloves while handling hot or cold samples.
- ▶ Wear protective gloves when working around the VT probe.
- ▶ Only trained personnel should be working with the VT probe system.

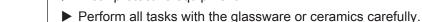
2.6.3 Safety When Working with Glassware

MARNING

Danger of injury from glassware or ceramics breakage!

Broken glassware or ceramics may cause minor injuries or material damage, but may also result in a life threatening situation if hazardous substances are used.

- ▶ If glassware or ceramics breaks, refer to the corresponding precautions and cleaning/ disinfection instructions.
- ▶ Wear protective equipment.



- ▶ Before carrying out any maintenance work, remove the samples and use dummy samples if necessary.
- ▶ Strictly observe the correct sample adjustment, i.e. the maximum sample height.
- ▶ Always transport the glassware or ceramics with the cover, if applicable. Never turn the glassware or ceramics upside down or on it's side.
- ► The laboratory supervisor is responsible for:
 - ⇒ Establishing and enforcing standard sample handling and cleaning procedures.
 - ⇒ Establishing and enforcing the use of protective clothing and equipment.
 - ⇒ Training laboratory personnel.
 - ⇒ Preparing an emergency plan.

3 Transport, Packaging and Storage



Installation, initial commissioning, retrofitting, repairs, adjustments or dismantling of the device must only be carried out by Bruker Service or personnel authorized by Bruker. Damage due to servicing that is not authorized by Bruker is not covered by your warranty.

3.1 Symbols on the Packaging

The following symbols are affixed to the packaging material. Always observe the symbols during transport and handling.

| Тор | <u> </u> | The arrow tips on the sign mark the top of the package. They must always point upwards; otherwise the content may be damaged. |
|--------------------------|----------|--|
| Fragile | I | Marks packages with fragile or sensitive contents. Handle the package with care; do not allow the package to fall and do not allow it to be impacted. |
| Protect Against Moisture | 7 | Protect packages against moisture and keep dry. |
| Attach Here | Q | Lifting gear (lifting chain, lifting strap) must only be attached to points bearing this symbol. |
| Center of Gravity | + | Marks the center of gravity of packages. Note the location of the center of gravity when lifting and transporting. |
| Weight, Attached Load | | Indicates the weight of packages. Handle the marked package in accordance with its weight. |
| Permitted Stacking Load | kg max | Indicates packages which are partially stackable. Do not exceed the maximum load-bearing capacity specified on the symbol in order to avoid damaging or destroying the content. |

Transport, Packaging and Storage

| Do not Damage Air-tight Packaging | | The packaging is air-tight. Damage to the barrier layer may render the contents unusable. Do not pierce. |
|--|---|---|
| | | Do not use sharp objects to open. |
| Component Sensitive to Electrostatic Charge | | The packaging contains components which are sensitive to an electrostatic charge. |
| | | Only allow packaging to be opened by trained personnel. |
| | | Establish potential equalisation before opening. |
| Protect from Heat | 淡 | Protect packages against heat and direct sunlight. |
| Protect from Heat and Radioactive Sources | 淡 | Protect packages against heat, direct sunlight and radioactive sources. |

Table 3.1: Symbols on the Packaging

3.2 Inspection at Delivery

Upon receipt, immediately inspect the delivery for completeness and transport damage.

Proceed as follows in the event of externally apparent transport damage:

- Do not accept the delivery, or only accept it subject to reservation.
- Note the extent of the damage on the transport documentation or the shipper's delivery note.
- · Initiate complaint procedures.



Note: Issue a complaint in respect to each defect immediately following detection. Damage compensation claims can only be asserted within the applicable complaint deadlines.

3.3 Packaging

About Packaging

The individual packages are packaged in accordance with anticipated transport conditions. Only environmentally friendly materials have been used in the packaging.

The packaging is intended to protect the individual components from transport damage, corrosion and other damage prior to assembly. Therefore do not destroy the packaging and only remove it shortly before assembly.

It is recommended to store the packaging for later use in the event that you need to return the unit to Bruker.

Handling Packaging Materials

Dispose of packaging material in accordance with the relevant applicable legal requirements and local regulations (see *Dismantling and Disposal* [65]).

3.4 Storage

Storage of the Packages

Store the packages under the following conditions:

- · Do not store outdoors.
- · Store in dry and dust-free conditions.
- Do not expose to aggressive media.
- · Protect against direct sunlight.
- · Avoid mechanical shocks.
- Storage temperature: 15 to 35 °C.
- Relative humidity: max. 60%.
- If stored for longer than 3 months, regularly check the general condition of all parts and the packaging. If necessary, top-up or replace preservatives.



Note: Under certain circumstances, storage instructions may be affixed to packages which expand the requirements specified here. Comply with these accordingly.

Transport, Packaging and Storage

4 Introduction

The minispec mq-one is a benchtop Nuclear Magnetic Resonance (NMR) analyzer for detection of hydrogen (¹H). Its common application is in polymer, chemical and of course in food industry quality control and quality assurance (QC/QA), where it is routinely used for fast, reproducible and non-destructive analysis.

This manual provides instructions on proper installation of the minispec mq-one and an introduction to the use of the minispec hardware and software. Topics covered include:

- Installation of hardware (section *Installation of the minispec mq-one Series* [27]).
- Switch-On [27].
- mq-one Start-Up [▶ 38].
- Running minispec Plus Software [43].

Once installation and configuration is complete, the user will benefit from the software introduction to familiarize themselves with the minispec capabilities. For installation procedures you may also refer to the latest version of the Pre-Installation manual(s) (booklet or other format).

Finally, for a better understanding of the principles involved, an introduction to the basics of NMR is provided in section *Basic NMR Principles* [> 59]. A minimum set of NMR parameters is described in *NMR Parameters* [> 61].

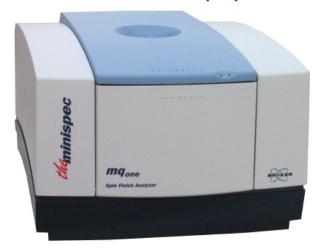


Figure 4.1: minispec mq-one Spin Finish Analyzer

The minispec mq-one Analyzers operate with the **minispec Plus** software, which is delivered with the system. This is a modern software package and there are separate manuals available on the minispec software CD that explain the operation of the software in all details:

- minispec Plus Administration
- · minispec Plus Classic
- minispec Plus Chemometrics

The **minispec.exe** software is the data acquisition software, running in the background of minispec Plus. However minispec.exe is mainly used for diagnostic purposes / service on the mq-one systems.

4.1 Improvements

The minispec mq-one Series is the sixth generation of benchtop pulsed NMR analyzers produced by BRUKER. Since the first BRUKER minispec series was introduced in the early 1970's, there have been many improvements in hardware and software. Highlights of the new mq-one Series minispec generation include:

- mq-one minispec systems are dedicated to certain minispec Standard applications and are perfectly tailored to those applications.
- minispec control and user interface software operates under Windows™ 7 32-bit/64-bit.
- Export functions, like Microsoft Excel export.
- Data integrity and 21 CFR Part 11 compliance.
- Highest reproducibility / all electronics are perfectly temperature stabilized in the mq-one housing.
- · Lowest noise generation combined with lowest energy consumption.
- · Compact design.
- Accessories as needed for the dedicated application are already delivered with the system.



Note: Some of the features/accessories mentioned above may be optional.

4.2 Siting Considerations

Place the unit on a strong, level, non-magnetic benchtop surface, capable of supporting the weight (refer to Weights and Dimensions). A minimum distance of 10 cm should be allowed between the back of the Analyzer Unit and adjacent objects in order to ensure sufficient aircooling.

Since magnetic objects containing for example iron can influence the magnetic field inside the Analyzer Unit, do not locate the system within 1 m of large magnetic objects or within 2 m of moving metallic objects.

A CAUTION



Accident or material damage hazard from falling or tilting instrument

Instrument may fall down or tilt during installation, retrofitting, dismantling, or while moving on a cart.

- ▶ Use the carrying handles during lifting.
- ▶ When a table or cart is used, it should meet the requirements in the site planning guide.
- ▶ The instrument should be secured to the cart or table.



Figure 4.2: mq-one Spin Finish Analyzer on a Strong Table

4.2.1 Environmental Considerations

The minispec should be used in areas free from direct sunlight, heat sources and power cables.

A constant temperature is important for field stability and accurate reproduction of measurement results.

The usual magnet temperature (if not indicated different) is 40°C for all instruments. Exceptions are:

mg-one Polymer Analyzer: 50°C

These temperatures have been selected because they are well above the expected ambient (laboratory) temperatures and therefore allow accurate tempering of the minispec unit.

Tempering of the magnet and the console electronics is accomplished with a closed cycle zero maintenance, air ventilation system, so that no external air is ventilated through the console or the Analyzer Unit.

In some factory environments where dust may be a problem, it may be desirable to house the minispec computer in a clean room or ventilated housing, which is protected from dust. The Analyzer Unit can be placed nearby at a location more convenient for process personnel.

The instrument contains strong magnetic fields, some of which extend beyond the Analyzer unit housing (see stray field diagram page 14-17). These pose no danger to routine users, but are hazardous to persons with heart pacemakers or other medical implantations.

MARNING

Risk to life due to high magnetic fields

A magnetic field of more than 0.5 mT (5 Gauss) is life-threatening for people with pacemakers or active metal implants. Exposure to more than 8 T can cause damage to health. Duration of exposure (8 h/day) above the limit of 200 mT can cause damage to health. Ferromagnetic tools in the magnetic field are significantly hazardous. Disks and electronic devices may be damaged.

- ▶ Mark the magnetic field of more than 0.5 mT (5 Gauss) before start up.
- ► Keep people with active medical implants or heart pacemakers away from the 0.5 mT (5 Gauss) area.
- ▶ The permanent workplace of employees must be outside the 0.5 mT (5 Gauss) area.
- ▶ Do not stay or work at magnetic fields of more than 8 T.
- ▶ Prevent exposure of more than 200 mT for more than 8 h/day.
- ▶ Keep disks, credit cards and electronic devices away from the identified area.
- ▶ Do not use ferromagnetic tools or items within the identified area.
- Only use non-ferromagnetic transportation dewars or pressure cylinders for the cryogenic agents.
- ▶ Only use non-ferromagnetic ladders or steps.
- ▶ Remove magnetic items (jewelry, watches, pens etc.) before carrying out maintenance work.

MARNING

Danger of injury or material damage due to strong magnetic fields!

Injury or material damage may result due to the strong magnetic fields that can draw metallic objects towards the magnet.



- ▶ DO NOT locate the instrument next to large iron-containing objects or near moving metallic objects.
- ▶ DO NOT place any iron-containing object on the minispec magnet unit. Be aware that the magnetic field can erase magnetic recording media such as computer diskettes or credit cards.
- ▶ DO NOT place these items or clothing containing these items on the magnet unit.
- Leave the dust cover on the probe canal when the instrument is not in use.



4.3 Unpacking the System

All manuals and accessories are packed in the container with the minispec. When unpacking the instrument ensure that all components listed in the packing list are part of the delivery.

⚠ CAUTION

Danger of property damage due to improper handling.



The shipping container must remain in an upright position at all times. It has two compartments separated by a wooden plate: an upper part, which contains the PC system, and a lower part containing the Magnet Unit. The magnet unit is secured to the shipping container from below with four bolts or may also be positioned in the shipping container with damping materials below the main unit. The packing may vary due to different accessories which may have been added to the shipment.

▶ DO NOT tilt the container when removing these bolts.

A CAUTION

Accident or material damage hazard from falling or tilting instrument

Instrument may fall down or tilt during installation, retrofitting, dismantling, or while moving on a cart.

- ▶ Use the carrying handles during lifting.
- ▶ When a table or cart is used, it should meet the requirements in the site planning guide.
- ▶ The instrument should be secured to the cart or table.

A CAUTION

Risk of injury from lifting heavy objects.



The unit is very heavy and may lead to injury when lifting.

- ▶ Do not attempt to lift the unit over the edge of the carton, remove the carton first.
- ▶ Do not attempt to lift the unit on your own or without necessary precaution against injury.
- Use a hoist if available.
- ▶ Follow the step-by-step instructions in the installation section of this manual.

To unpack the system:

- 1. Use a 13 mm wrench to remove the four bolts from the bottom of the container (if fixed this way).
- 2. Remove the shipping straps and open the container.
- 3. Remove the packing material from around the PC system.
- 4. Remove the PC system from the container, together with the wooden plate that it is mounted on (do not tip!).
- 5. Remove the packing material from around the Analyzer Unit. Remov the retaining screws or nails from the bottom of the wooden pallet and **detach** the shipping carton. Depending on packing, the procedure may need to be adapted accordingly.
- 6. While keeping it level, carefully lift the Analyzer Unit from the pallet using the handles on either side, and place it on a sturdy cart or benchtop.



When using a hoist, make sure the straps are capable of carrying the Analyzer's weight (up to 150 kg) and are attached in such a way that the unit cannot fall, slip, topple or turn while being carried.

7. Once the system has been placed on the bench in the desired position, the handles can be removed. Use an adequate Allen keys to remove the screws (totally 8 screws) and remove the handles and bars. Store bars, handles and screws on a safe place so that it can be re-installed at a later time (if needed).



Figure 4.3: Handles on the Side of the Magnet Unit

- 8. Remove and retain the clear plastic dust cover from the minispec unit and inspect it for damage.
- 9. If any item appears to be damaged, contact your BRUKER representative immediately.



Note: Depending on the accessories / consumables ordered, packing may vary.

4.4 Installation of the minispec mq-one Series

In general, the minispec mq-one Series consists of one (two) units:

- Analyzer Unit, containing the magnet system, the probe assembly and all electronics
- Standard PC with user interface (GUI) for measurement control, data processing, etc.



Figure 4.4: The minispec Analyzer Unit (left) and the PC System (right).

A number of optional accessories can be added and adapted for use: Electronic balances, auto sampler, temperature control baths etc. Bruker also offers SFC Automation systems complete with tempering devices (Peltier technology) and barcode readers.

4.4.1 Analyzer Unit Connections

The connectors are located on back of the instrument. Connect the unit as shown in the figure below:



Figure 4.5: Connections on the Back of the Analyzer Unit

| 1. | Ethernet connection | | | |
|----|---------------------|--|--|--|
| 2. | Main switch | | | |
| 3. | Main power input | | | |

4.4.2 Switch-On

Assuming all the cables on PC and minispec mq-one are connected, switch on both systems. The mq-one boot up procedure may take a couple of seconds.

The mq-one shall show a blue left LED (power ON) and a red right LED (system in warm-up phase). The mq-one will need several hours (4-6) to warm-up. After this time the right mq-one LED will have switched to blue, too – indicating that the system is on temperature and is ready to be operated.

It is recommended to let the mq-one Analyzer run permanently – if there is no special reason it should always remain switched ON. Consumption of electricity is low (comparable to an energy saving lamp).



Figure 4.6: mq-one Polymer Analyzer after Switch-On

4.5 Interpretation of the LEDs

Users receive continuous indication of the status of the Analyzer unit in the form of light emitting diodes (LEDs), which are built into the front panel of the unit.

mq-one Analyzer Unit

Right LED, indicates the magnet temperature status:

- RED: Pre-heating
- · Purple: Transition to normal heating
- · BLUE: Temperature is OK

Left LED, power indication.

4.6 Calibration Sample and Probe Exchange

The Analyzer Unit cover has two outer hatches or doors.

- The first one is on the front panel of the unit and can be used to contain the calibration/ Daily Check samples. Pressing on the upper part of the hatch will unlock and open it. The 10 and 18 mm calibration samples can be stored, but larger diameters cannot be stored in this door.
- The second is the top hatch, which allows access into the minispec magnet/electronics compartment and permits quick and tool-free exchange of the minispec probe.



Figure 4.7: minispec mq-one SFC Analyzer with Both Latches Unlatched

Remark: The mq-one Seed XL Analyzer has the front panel door always in the "open" position and the top hatch is not latched to the unit, but just lies on top of the housing.



Figure 4.8: mq-one Seed XL with the Lower Latch in the Open Position (normal state of operation)

To replace a probe you must open the hatch at the top of the magnet unit.

- 1. This is done by first releasing the front hatch to expose a red button in the front of the unit.
- 2. Press the red button to release the top latch and open the hatch as far as it will go.
- 3. A second hinged lid, blue in color, will be visible. Lift it up and lean it against the outer hatch.
- 4. See the above remark for the mq-one Seed XL system.

WARNING



Danger of injury due to falling lid

The hinged lids may close unexpectedly during probe exchange causing injury to hands or fingers.

- ▶ Ensure that the gas spring on the outer lid is operating correctly.
- ▶ The blue inner hinged lid does not have a gas spring, use extreme care when exchanging the probe assembly.
- 5. The probe assembly is fixed with two quick-release fasteners. To release the fasteners, lift up the D-rings until they snap into a vertical position, then use them to rotate the fastener posts until released (refer to the figure below).
- 6. While grasping the D-rings, carefully tug upward to loosen the preamplifier connection under the mounting plate, then raise the assembly (mounting bar with probe and preamplifier attached) out of the magnet gap. In some systems (like the mq-one SFC) the preamplifier is not attached to the probe, but it is fixed separately on the magnet yoke.

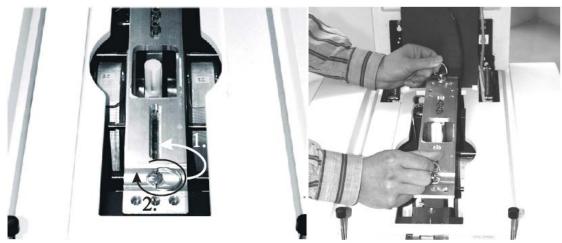


Figure 4.9: Ring of the Quick-Release Fastener (left) and the Raising of the Probe Assembly (right)

| 1. | Rings | | | | |
|----|--|--|--|--|--|
| 2. | Rotating the rings. | | | | |
| | To open the fasteners, turn the rings (1) upward and rotate them (2) | | | | |

Replace the assembly by following the instructions in reversed order.

Intelligent probes were developed for the minispec Series. If you exchange a probe the software will read the most important parameters (pulse length, resonance frequency) from the probe itself. The software will prompt the user to confirm the settings. For fine-tuning, it is recommended running the **Update Settings** procedure afterwards.

Probe exchange for **mq-one analyzers** is typically not meaningful for this product as only one type of probe can be used for each mq-one Analyzer. It might be needed to swap 2 equal probes for service work, however for this type of analyzer, Bruker recommends only trained and authorized personnel be allowed to exchange probes if necessary.

5 Technical Data

5.1 General Information

| No. | Series | Туре | Weight (kg) | Length (cm) | Width (cm) | Heigth (cm) |
|-----|--------|-------------|-------------|----------------|---------------|----------------|
| 1 | mq-one | SFC | 95 | 65 | 50 | 33 |
| 2 | mq-one | Polymer | 130 | 65 | 50 | 33 |
| 3 | mq-one | Fat | 130 | 65 | 50 | 33 |
| 4 | mq-one | Spin Finish | 130 | 65 | 50 | 33 |
| 5 | mq-one | Hydrogen | 130 | 65 | 50 | 33 |
| 6 | mq-one | Seed | 130 | 65 | 50 | 33 |
| 7 | mq-one | Seed XL | 150 | 65 | 50 | 33 |

Table 5.1: Technical Data: General Information

All specifications above are without a PC. Weights and dimensions apply to the instruments, not to the packaged systems.

5.2 Connection Values

Grounding is vital for the safe operation of the instrument. Never operate with the grounding conductor disconnected. If the local wiring does not provide a ground, an earth-to-chassis connection must be added at the user's location.



Note: Since the input voltage may be unstable in a laboratory environment, it is recommended to connect the minispec to a separate circuit that is not used by any other equipment. Furthermore, a voltage stabilizer or UPS may be required to avoid instrument instabilities or other unexpected system behavior caused by a fluctuating input voltage.

| No. | Series | Туре | Voltage/VAC | Apparent Power Consumption, Maximum/VA | Circuit Protection (Two indications: NF/ND Series) | Frequency/Hz |
|-----|--------|-------------|-------------|--|--|--------------|
| 1 | mq-one | SFC | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |
| 2 | mq-one | Polymer | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |
| 3 | mq-one | Fat | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |
| 4 | mq-one | Spin Finish | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |
| 5 | mq-one | Hydrogen | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |
| 6 | mq-one | Seed | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |
| 7 | mq-one | Seed XL | 100-240 | 180 | 2.5 AT (2 pieces) | 50-60 |

Table 5.2: Electrical Connection Values

5.3 Operating Conditions

Environment

| No. | Series | Туре | Temperature Range, Maximum/°C | Temperature Range, Ideal/°C | Relative Humidity at 31 °C, Maximum/% | Decreasing Linear Till Relative Humidity < 50% at 40°C, maximum/% | IP Safety Class |
|-----|--------|----------------|-------------------------------------|--------------------------------|--|--|-----------------------|
| 1 | mq-one | SFC | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |
| 2 | mq-one | Polymer | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |
| 3 | mq-one | Fat | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |
| 4 | mq-one | Spin Finish | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |
| 5 | mq-one | Hydrogen | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |
| 6 | mq-one | Seed | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |
| 7 | mq-one | Seed XL | 18-28 | 22-25 | 80 (non- condensing) | < 50% | IP20 |

Table 5.3: Operating Environment

Normal environmental conditions (CAN/CSA 61010-1-12; IEC 61010-1: 2010; ANSI/UL 61010-1)

- · Indoor use only.
- · Maximum operation altitude: 2000 m.
- Ideal operating temperature: 22-25 °C. Minimum operating temperature: 18°C Maximum operating temperature: 28°C Humidity (non-condensing): 20-80%
- Maximum relative humidity 80% for temperatures up to 31 or decreasing linearly to 50% relative humidity at 40 °C.
- MAINS supply voltage fluctuations up to $\pm 10\%$ of the nominal voltage.
- TRANSIENT OVERVOLTAGES up to the levels of OVERVOLTAGE CATEGORY II.
- · Pollution degree 2.
- · Protection class IP20.

5.4 minispec Software CD

| Description | Manual | Bruker Part Number | | | |
|---|---|-----------------------|--|--|--|
| minispec Software CD-ROM (Windows 7/Office 2010*). | The minispec Pre-Installation manual is available as a PDF document on this CD-ROM. | E1405284 | | | |
| * Note: It is planned to switch to Office 2013 by the middle of 2015. | | | | | |

Table 5.4: Bruker minispec Software-CD

5.5 Rating Plate

The rating plate is located at the power input and includes the following information:



Figure 5.1: The minispec mq-one Series Rating Plate

Technical Data

6 Getting Started

6.1 List of Standard Applications

With the minispec mq-one series, nearly all standard applications are executable. The most common applications are listed in the following:

mq-one SFC Analyzer

 Solid fat content determination in fat compositions (SFC) using solid fat content (ratio) calibration standards with Bruker certificates (ISO 8292-1 / 8292-2; AOCS Cd 16b-93)*

mq-one Fat Analyzer

- · Oil/Fat & Moisture in
 - Chocolate
 - Cocoa powder
 - Milk powder

mq-one Seed Analyzer/mq-one Seed Analyzer XL

- · Oil & Moisture in
 - Seeds/residues/press cake (ISO 10565 / 10632; AOCS Ak 4-95)*
 - Nuts
 - Olives

mq-one Polymer Analyzer

- · Polymer Analysis like:
 - Xylene soluble content in polypropylene
 - Additive determinations in polymers
 - Polybutadiene / polystyrene content in SBR
 - Density in polyethylene
 - Crystallinity determinations in polymers

mq-one Spin Finish Analyzer

· Spin-finish determinations (OPU) on man-made fibers

mq-one Hydrogen Analyzer

- · Total hydrogen content determinations in hydrocarbons like
 - Jet fuel (ASTM D7171)*
 - Other distillates

^{*} International Standard Methods apply for these applications.

6.2 mq-one Analyzers and Accessories

The minispec mq-one Analyzers are not delivered as an analytical spectrometer only, but are also provided with a set of additional accessories / consumables as needed for the specified application field of the analyzer.

The following table below shows the accessories / consumables accompanying the various mq-one systems:

| Analyzer | Addition1 | Addition 2 | Addition 3 |
|--------------------|---|--|---|
| mq-one SFC | Set of 3 Bruker SFC | Package of 10 mm Sample | |
| | Calibration Standards | Tubes with caps | |
| mq-one Polymer | Set of 3 Bruker SFC | Package of 10 mm Sample | Aluminum Block for 10 mm Sample |
| | Calibration Standards | Tubes with caps | tubes (fits into metal block |
| | | | thermostats) |
| mq-one Fat | Easyfill 18 mm Sample | Aluminum Block for 18 mm Sample | |
| | Tubes | tubes (fits into metal block thermostats) | |
| mq-one Spin Finish | Glass-free 18 mm sample | Aluminum Block for 18 mm | Set of Spin Finish Calibration |
| | Tubes (no proton signal) | Sample tubes (fits into metal block | Transfer / Validation Samples |
| | | thermostats) | |
| mq-one Hydrogen | Package of 18 mm Sample Tubes with caps | Plugs for 18 mm Sample Tubes (avoid sample evaporation) with | Aluminum Block for 18 mm Sample tubes (fits into metal block |
| | | one Rod | thermostats) |
| mq-one Seed | Package of 40 mm Sample Tubes with caps | Aluminum Block for 40 mm Sample tubes (fits into metal block thermostats) | Set (3) of Rape seed material for instrument calibration |
| mq-one Seed XL | Package of 50 mm Sample Tubes with caps | Set (3) of Rape seed material for instrument calibration | |



Figure 6.1: mq-one Spin Finish Analyzer with Glass-Free Sample Tubes

All systems are furthermore accompanied by a suitable Daily Check sample or in the case of the mq-one SFC/mq-one Polymer analyzer a set of 3 Bruker calibration standards.



Figure 6.2: Example of a Daily Check Sample (here for mq-one Seed XL Analyzer)



Figure 6.3: Easy-fill 18 mm Sample Tubes for the mq-one Fat Analyzer

6.3 mq-one Start-Up

In general, minispec mq-one systems are delivered with a personal computer and have the minispec software already fully installed. In this case, the user can skip the software installation instructions (see *Software Installation* [38]). In case the PC and mq-one have been directly connected with the blue connection cable, proceed with *Running the minispec mq-one* [43].

In case the customer wants to connect PC and minispec to his local network, please proceed to *Direct Cable Connection* [39] before switching to *Connection of PC and minispec mqone via a Network* [40].

When a user provides his own personal computer, or if software needs to be reinstalled for use with the minispec, refer to the installation instructions below.

For details on running minispec.exe, please note that this software is typically not used by the mq-one users. Only in exceptional cases – mainly for service purposes – the minispec.exe software is used.

There is a separate chapter on the mq-one software: the minispec Plus software. This manual gives a brief introduction of the use of the minispec Plus software. For further details, the mq-one SOPs may be visited and of course also the dedicated minispec Plus manuals for Administration, Classic applications, and Chemometrical analysis.

6.4 Software Installation

Execute the following steps only if the PC has not been pre-configured for the minispec.

- 1. Insert the installation CD in your drive.
- 2. Open the Windows EXPLORER and check the CD for a ReadMe.txt file. If a ReadMe.txt file is available, follow the instructions provided in this file.
- 3. If not, execute the Setup file with a double click or select the setup entry with the right mouse button and select **Open** in the displayed menu.
- 4. Follow the instructions in the Setup program.
 - The Setup program copies the files into the folder you specify during the setup procedure.
- 5. To start the minispec.exe software, double click on the minispec.exe file in the main folder. Alternatively, you can create a shortcut on the Windows desktop to the file minispec.exe.

With the first start up, the configuration of the minispec software (minispec.exe) is set to the QC-Analyzer.

The mq-one instruments operate with the minispec Plus software, with the above described minispec.exe software running in the background as an acquisition server. Systems that are equipped with minispec Plus software will install this additional program automatically. The manual *minispec Plus Administration*, together with the other minispec Plus manuals, provide further details. These can be found on the minispec software CD in the folder *Documentation*.

Systems equipped with minispec Plus software do not necessarily need to start the minispec.exe software before using minispec Plus. If the system is properly installed (refer to the corresponding minispec Plus manual), then minispec Plus can be opened without first opening the minispec.exe software. However in some cases it might be useful to first run the minispec.exe software to make sure there is a proper network connection from PC to the minispec, then afterwards switch to minispec Plus program.

Please note that for proper installation of minispec Plus software further software requirements may apply, refer to the corresponding minispec Plus manual for details.

6.5 Connecting the PC to the minispec for the First Time

6.5.1 Direct Cable Connection

In the normal case the minispec mq-one and the PC were delivered together from the factory. Then the minispec software has already been installed on the computer and the proper connection between PC and minispec has been already established and double-checked before. Only if this is not the case or the customer plans to attach the minispec PC to his network, then the following instructions are of importance.

- 1. If the software is running (e.g. after installation), then exit the minispec software.
- 2. Connect the PC to the minispec using the blue crossed-wire UTP-cable, which is delivered with the minispec (10-Base-T with RJ45 connectors, see the figures in the section *Installation of the minispec mg-one Series* [> 27]).

If not already installed, use the **Network** entry in the Windows[™] **Control Panel** to install a TCP/IP protocol on your PC. The exact procedure for adding the TCP/IP protocol depends on the Windows version that is used, refer to the Windows software documentation for a detailed description.

- 1. Select **TCP/IP Properties**. Confirm or enter the following entries: IP-address: 192.168.1.2 Subnet-mask: 255.255.255.0
 - If other values are defined, alter them accordingly. Re-boot your computer.
- 2. Start the minispec software on the PC.
 - Some program information will be displayed for a short time, after which a Welcome Box will be displayed. Entries in the select boxes indicate how the PC will attempt to connect to the minispec console and what applications will be loaded.
- 3. Connect to the minispec unit (mq-one Series) using the indicated default serial number NE0000 by clicking **OK** in the displayed *Welcome Box*.
 - Communication is attempted from the PC software over the TCP/IP to the CPU/ Ethernet controller in the console at the default IP address 192.168.1.200. Connection is indicated at the top status line with the message, for example, **Connected to NE3000**. The IP address of the console will be displayed in a small box on the bottom edge of the program window.
 - If the connection with the default serial number NE0000 cannot be established, re-try using the IP address '192.168.1.200' instead of the default 'NE0000' from the Welcome box settings.
- 4. If the connection still fails, make sure the cable is a crossed-wire twisted pair cable and that it is connected properly.
 - If connection still does not succeed, then the problem may be due to incorrect IP addresses or Subnet mask for the PC or the minispec. Normally the minispec console is shipped with the default IP address set to 192.168.1.200 and a subnet mask of 255.255.255.0. However, in some circumstances the minispec console may be set to other values (e.g. if a minispec has already been installed on a network, whereas another IP address will be needed, or a PC is being exchanged, or the software had to be reloaded on a fresh hard disk).
- 5. If a connection cannot be established and the setting of the console IP address is suspect, it may be necessary to reset the IP address into the mq-one electronics. The Internet web browser page contains information (see **Help** menu) on how to do this, however please check with your local Bruker support for more details, if necessary.

6.5.2 Connection of PC and minispec mq-one via a Network

- Ask the network administrator to assign unique and valid IP addresses for the PC and the minispec mq-one.
- Establish a direct connection as described in the section *Direct Cable Connection* [▶ 39] and exit the minispec software after the connection procedure has been completed successfully.
- To set the minispec console IP address from the PC, proceed as follows:
- 1. Open the Internet Explorer of your Windows OS on your PC.
- 2. Type the default address 192.168.1.200 in your browser to connect to the mq-one.
- 3. Windows security will prompt for a User Name and a password. Use "root" as a User Name and "BRUKER" as your password.
 - You should now have access to the main menu.
- 4. Select **Support** and afterwards **Network parameters**.
- 5. Set the new IP address and type on Apply Changes.
- 6. Re-boot the analyzer to activate the new address.
- 7. Modify the IP address/network parameters on the PC side too. It may be required to reboot the PC.
- 8. If you change the cable connection, for example, if you connect the PC and minispec to the network, make sure that you use the correct communication cable, as cables for direct and indirect communication may differ.
- 9. Connect the PC and minispec via the network using minispec.exe software. In case of problems, Bruker authorized service may be contacted.
- 10. Assuming the connection to the minispec via minispec.exe software was successful, close the minispec.exe software and switch to minispec Plus software. You may then proceed to *Running the minispec mq-one* [> 43].

6.6 minispec mq-one Systems Software GUI

As indicated before, the mq-one systems are intended to be operated using Bruker's minispec Plus software GUI. The **Update Settings**, **Daily Check**, **Calibration** and **Measurement** procedures are also included in both the minispec exe and minispec Plus software, but when minispec Plus software is available it is recommended to operate those systems using this software.

Because all the applications and calibrations are prepared for the user using the minispec Plus software, the application pool for minispec.exe, known from the mq-Series systems, will not be installed on mq-one systems. It is also not possible to copy mq-Series applications to mq-one systems, as the pulse sequence programming differs slightly for both systems. For minispec Plus users, the minispec.exe will only be used in a few exceptional cases, including:

- Checking the connection between PC and minispec system in some cases.
- · For diagnostic purposes.

Service technicians may use the minispec.exe software on mq-one systems more frequently.

6.7 minispec.exe Software: Quick Hands-On

As the minispec.exe is used for diagnostic/service purposes, as well as to test the connection between the PC and minispec mq-one, a very brief introduction is provided here.

6.7.1 minispec.exe Software: Wake-Up State

When the minispec.exe software starts, a general dialog is displayed concerning the software version and the copyright. Then a *Welcome Box* opens and displays information about the configuration of the system. The wake-up configuration is the configuration used with your last minispec session. To continue with the same settings and start the minispec software click **OK**. If you want to change the settings refer to the next section, *Configuration and Welcome Box* [67].

6.7.2 minispec.exe Software: General Handling

The most important commands that are used to control measurements are: the **Run** command to start a measurement and the **Stop** command to interrupt a measurement in progress. Measurements can be started through a number of commands and by activating a number of software icons or features. For example, the general Run command can be started through the RUN button from the top icon bar or bottom button panel, from the pull-down menu **minispec**, or by simply pressing **<Enter>**. If the user has been given permission to perform sample calibrations, then the **Calibrate** command is available. Other forms of measurement are available for convenience, including a repetitive run etc.

Getting Started

7 Running the minispec mq-one

7.1 mq-one On Temperature

Once both LEDs on the mq-one have switched to blue, the system is ready to run.

The PC that has been started will pause at the Windows log-in window. When configured by the factory, no password has been entered and the user may proceed by pressing **Enter**. The PC will then finish the boot-up process and show the minispec Plus icon on the desktop. Besides the software icon, a link to the "minispec documentation" folder is also on the desktop.

7.2 Running minispec Plus Software

Double-click on the minispec Plus icon to start the software. The software will start and come to the log-in screen.



Figure 7.1: The minispec Plus Log-in Dialog

To get full access to all the menus of minispec Plus, type **ADMIN** and press the **Enter** button. You will now be transferred to the main menu of minispec Plus.

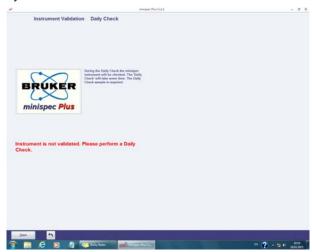
Running the minispec mq-one



Figure 7.2: The minispec Plus Main Menu

7.2.1 Daily Check

As a first action, chose to run the **Daily Check** function to validate the mq-one system. The software will now guide you through the procedure, requesting the Daily Check sample or the 3 SFC calibration standards. Insert the corresponding samples with care into your NMR system.

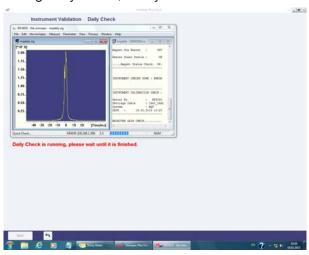


Finally the test should conclude and the instrument should be valid for 24 hours. In case there is a Daily Check failure, it is recommended to run the *Update Settings* procedure and to follow the corresponding instructions. In any case if the *Update Settings* routine does not run automatically, the Daily Check procedure has to be repeated.

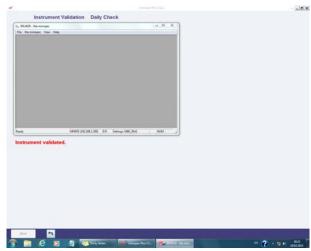


Figure 7.3: Operator Inserting the Daily Check Sample into the mq-one Analyzer

During Daily Check, the system runs a number of tests, all following one after the other.



If all the tests passed, the software will indicate this accordingly. The corresponding message will also be displayed in the main menu.



7.3 SFC Calibration

As compared to all the other instrument calibrations, SFC plays a special role in this respect. During the Daily Check procedure, the SFC values of the 3 Bruker standards are re-checked and in case the Daily Check passes, the system is already calibrated for SFC (Solid Fat Content) analysis.



Figure 7.4: Set of Bruker SFC Standards for Instrument Calibration and Check

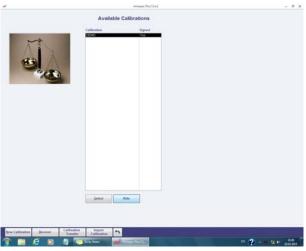
The user can then directly proceed to the **Measurement of unknown samples**. The minispec Plus software supports both, direct and indirect SFC methods although customers widely use the direct methods. Be aware to choose your method according to the International Standard method and according to the type of fat that is investigated.

7.3.1 Other Calibrations

For all other applications the customer will need to calibrate the system with his own reference standards. Typically 4-6 standards with known reference values are needed per calibration line. In most cases the mq-one Analyzers are calibrated in a classical way, i.e. the NMR signals of FID or Hahn-echo (or both) are considered and the corresponding amplitudes are correlated with the sample properties.

For different types of samples (like different types of oil seeds, polymers according to different production processes or different types of spin finishes) the user may need to create different calibration lines, one line per type of sample. It is recommended to name the calibrations accordingly.

The user may choose the Calibrate button and proceed to the Calibration menu.



Calibration Configuration

Californium Stance

Create a new calibration and select a corresponding name.

Choose the corresponding Bruker pre-defined method and double-check the number of scans.

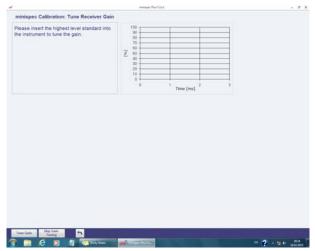


The user may also define a reference sample / standard that can be measured periodically by the instrument.

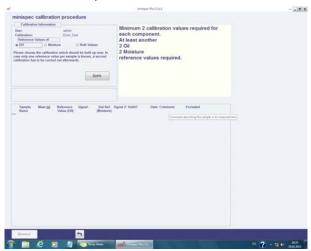


Running the minispec mq-one

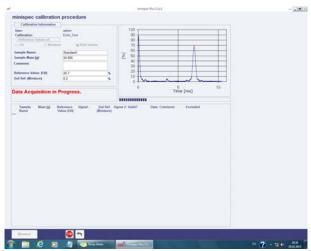
Start the calibration and tune the gain with the sample that has the highest NMR signal (typically the sample with the highest mass / highest concentration).



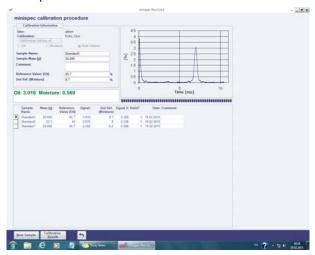
After Gain Adjustment one calibration sample after the other is analyzed. Depending on the application one or two parameters are calibrated. It is also possible to calibrate for 2 values simultaneously. Start with the first sample. As the Gain is fixed now, the order in which the calibration samples are measured does not matter.



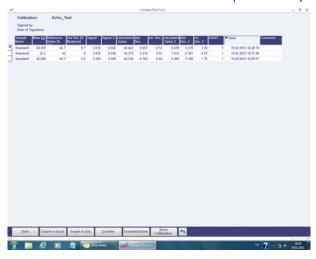
The calibration measurements are shown on the screen.



After the first sample is done, go on with further calibration samples. By default the software requests a minimum of 3 samples per calibration parameter (oil and moisture typically). However often the calibration can be imroved by including further samples, for example 5 or 6.

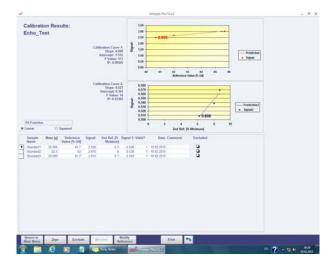


When the measurement of all the samples is completed, switch to the calibration results.



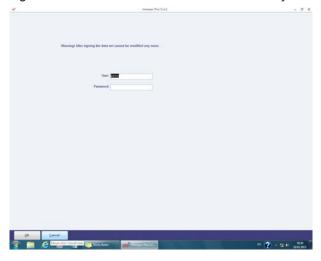
Afterwards move forward to the calibration line and inspect the correlation and other parameters describing the calibration quality.

Running the minispec mq-one



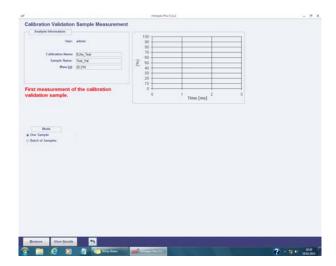
You might add samples or delete some, depending upon the needs and results of the calibration.

As the very last step and when the calibration fulfills the requirements, the calibration is signed. From then on it cannot be modified any further.

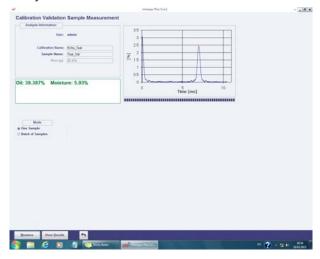


The only way to continue to work with this calibration is to make a duplicate of this calibration and also copying the calibration data points.

If the calibration is signed, one may leave the calibration section and switch to the Measurement part or the Calibration Validation measurements is executed. Here a defined sample is measured on a daily base and the results are recorded by the software for stability / performance check and also as a validation tool.



Once the Calibration validation measurement has completed, the result will be displayed on the screen and added to the list of Calibration Validation measurements for statistical analysis.



Running the minispec mq-one



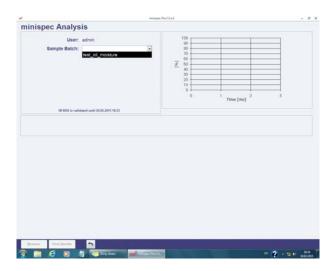
Figure 7.5: mq-one Spin Finish Analyzer with Set of Spin Finish Validation Samples

Afterwards switch back to the main menu of minispec Plus to start running measurements of unknown samples.

7.4 Measurements of Unknown Samples

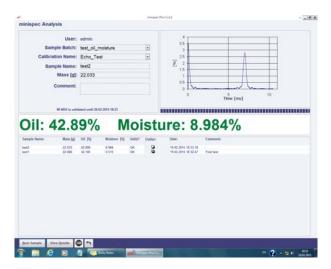
When the calibration(s) is(are) finished, one may switch to the "Measurement" section. Here unknown samples are analyzed and measured according to the calibration curve selected by the user.

• Enter the batch name of the sample to be analyzed.

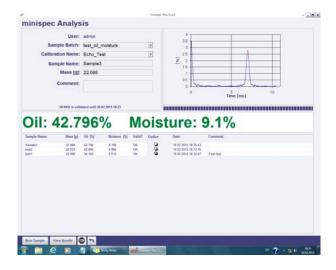


• Select the corresponding calibration method. Note: once batch and calibration are chosen, those are connected to each other. The software then remembers this connection when doing further measurements.

- Depending upon the method, as it has been defined during the calibration, the sample may need to be weighed. Enter the corresponding sample weight into the software or get the mass transferred from the balance connected.
- Insert the sample into the NMR as instructed by the software and see the measurement progress.
- Once the measurement has completed, the result will be indicated and displayed on the screen in large letters and also on the results list.

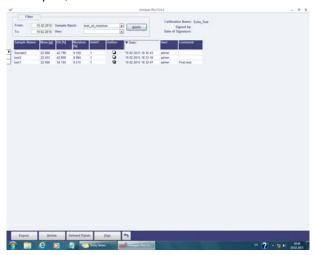


· Proceed with the next measurement or leave the Measurement menu.

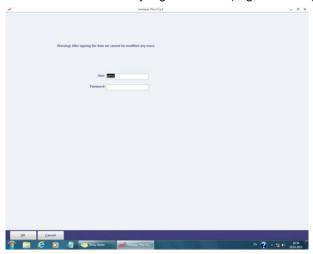


7.4.1 Result Handling

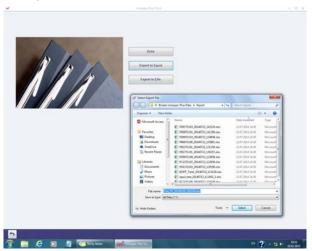
As unknown samples have been measured, the results are archived into the minispec Plus data base. Going to "Results" the data can be sorted / selected according to criteria such as time span, user etc.



Once selected one may sign the data (Sign function).



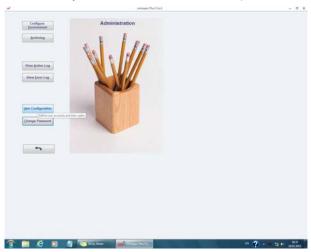
Or export data either to ASCII file or to MS Excel.



Exporting to MS-Excel templates are used so that the data is presented in the most clearly arranged way.

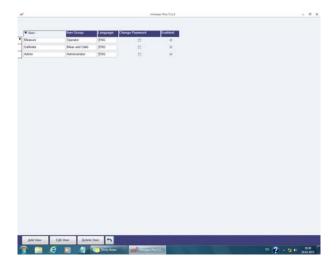
7.5 Administration Details

minispec Plus comprises an extensive Administration section. Also for this part counts: the most prominent features for your application should already be factory set and for most of the customers there will be no reason to access this part of minispec Plus. This part can only be accessed by an user with Administrator permissions.



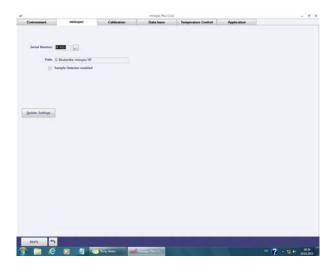
Not mentioned so far is the fact that minispec Plus runs with 3 permission levels:

- · Administrators with full access.
- User with "Calibration" permission having access to the Calibration and the Measurement parts.
- · User with "Measure" permission having access to the Measurement part.

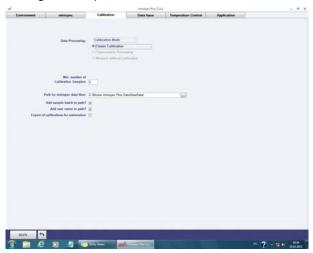


Moreover the minispec can be configured, please see the next screenshot. The minispec serial number as well as software installation path can be set. However – if the software runs for instance the Daily Check successfully, then there is no need to do any modification on those settings.

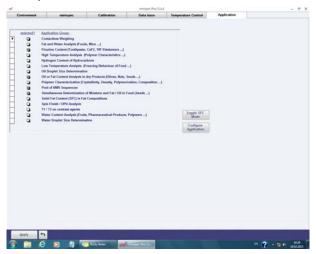
Running the minispec mq-one



Calibration settings can be specified in minispec Plus, for instance the number of calibration samples to be measured as a minimum – despite the below example, we recommend a minimum of 3 calibration samples per parameter to be analyzed. This is also the default setting in minispec Plus software.



Finally application settings can be defined in minispec Plus – we recommend to approach this only in case your designated application cannot be selected within the calibration section of minispec Plus.



7.6 More Details

For further details on the calibration procedures, measurements, results archiving, administration please refer to the dedicated minispec Plus manuals dealing with those matters in much more detail.

The following manuals exist:

- · minispec Plus Administration
- minispec Plus Classic Applications
- · minispec Plus Chemometric Applications

Also for each analyzer there exists an SOP (Standard Operating Procedure) that explains calibration and measurements, etc. tailored to the main application of the corresponding mq-one Analyzer.

Running the minispec mq-one

8 Basic NMR Principles

NMR (Nuclear Magnetic Resonance) is made possible by the properties possessed by some atoms that cause their nuclei (part of every atom) to have a magnetic moment. The atom most commonly investigated by NMR is Hydrogen (¹H), the nucleus of which is composed of a single proton. Hydrogen is present in many natural and synthetic substances like oil, water, polymers, pharmaceutics and foodstuffs. In a strong external magnetic field (called polarizing field) produced by the permanent magnets in the Magnet Unit, the magnetic moments can be oriented, and the vector sum of all moments results in a macroscopic magnetization. The amount of magnetization depends on the strength of the external magnetic field and the temperature.

Pulses of radio frequency (RF) at a suitable frequency can influence the magnetization in the sample. In NMR this resonance frequency, called Larmor frequency, depends on the field strength of the external magnetic field and the nucleus investigated. For example, at a field strength of 0.47 Tesla, protons (¹H) have a resonance frequency of 20 MHz. The orientation of the magnetic field generated by the RF pulse is perpendicular to the static external polarizing field.

When, for example, a sample containing NMR-active nuclei is exposed to a strong external magnetic field by inserting a sample into the sample orifice of the magnet, the process of buildup of macroscopic magnetization will start immediately, but it takes some time until the equilibrium is reached. The time constant of this built-up process is called longitudinal relaxation time T_1 (see figure).

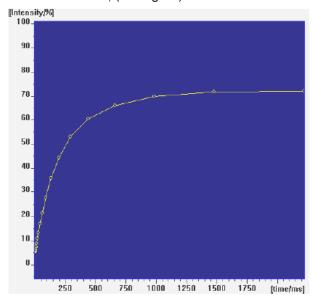


Figure 8.1: Increase of the NMR Signal Due to Longitudinal Relaxation

With skillful sequences of RF-pulses (generated by the minispec electronics and transmitted to the sample via the probe) the macroscopic magnetization can be influenced. One possibility is the generation of so-called transverse magnetization. This is not an equilibrium state, and therefore different relaxation processes arise. The transverse magnetization is still the vector sum of discrete atomic magnetic moments. Each one of these moments underlies a specific time evolution, and a loss of phase coherence results. The time scale of this magnetization loss is described by the transverse relaxation time T_2 (see figure) in the easiest case.

Basic NMR Principles

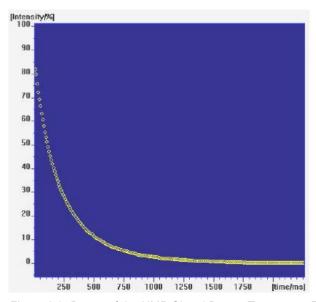


Figure 8.2: Decay of the NMR Signal Due to Transverse Relaxation

Secondly, the system naturally tends to relax back to the thermal equilibrium. This process is equivalent to the polarization process described above and takes place with the time constant T_1 . Various other processes are known from NMR-theory, depending on the pulse sequences used to manipulate the magnetization. These processes are described by different relaxation times, some examples are T_{1p} , T_{1D} , and T_{2e} .

Substances and materials can be characterized by relaxation measurements because the relaxation times are highly sensitive to molecular properties. For example, they can be sensors for various ranges of molecular motions. The large range of motions that can be characterized by NMR is a main point which makes NMR to such a valuable tool in analysis. For example, because of their different relaxation behavior solid and liquid parts in one sample can be distinguished clearly and their amount determined as in Solid Fat Content (SFC) measurements. As a consequence such materials as foodstuff, cosmetics, chemical products and much more can be investigated. For a more detailed description refer to the application descriptions available from Bruker.

Furthermore, the intensity of the NMR signal is a function of the number of atomic moments contributing to the macroscopic magnetization. Therefore, the signal is a measure of the number of nuclei in a sample. The minispec methods make use of this relationship to determine the amount of, for example, oil or moisture in a wide range of samples.

In summary, NMR makes use of the nuclei in substances as sensors of their surroundings, yielding important information about the matter. Since both excitation and detection are performed via electromagnetic waves in the radio frequency region, this analytical method is contactless, non-destructive, and rapid.

9 NMR Parameters

When defining the calibration/method in minispec Plus software, the software prompts typical values for the NMR sequence parameters. However, it might be necessary to adjust these parameters, especially if the method of test differs from the default approach. Then it is useful to adjust the NMR parameters accordingly.

In the following sections typical parameters that need to be set are explained in detail. The parameters Scans, Recycle Delay Time and Gain especially need to be adjusted or optimized. The parameters Dummy Shots and Acquisition Pre-Delay Time are used less often.

9.1 Scans

Scans is used to set the number of times the NMR experiment should be repeated for signal averaging before the result is evaluated. The required number of scans (possible range 1-32000, typically 1-512) depends on the signal strength, the desired signal-to-noise (which will limit the precision of the measurement), and the desired speed of analysis (time between scans is set by the Recycle Delay). Signal to noise improves with the square root of the number of scans. The remaining number of scans during an experiment is shown in the lower right corner of the display.

9.2 Recycle Delay Time

The RD, or **Re**cycle **D**elay time (given in seconds), is used to set the time delay in seconds between repeated scans. The recycle delay is usually set to 5 times the longitudinal relaxation time T_1 to ensure that the sample returns to the thermal equlibrium state after a scan. If the delay is deliberately made shorter than the sample relaxation time, one or more dummy shots can be made prior to the experiments in order to ensure that the first scan has the same history as all subsequent scans.

9.3 **Gain**

Gain sets the signal amplification in the receiver. For best results, set the gain such that the highest part of the signal reaches about 80% of the signal input range. In minispec Plus software the gain is adjusted automatically. The software will also indicate the allowed range.



Note that the gain should not be changed for calibrated applications. If the range of input signals is too large for one gain setting, it may be better to have several calibrations for different gain settings.

9.4 Acquisition Pre-Delay Time

In some cases a defined delay is desired between the time a sample is inserted and the time of measurement start (e.g. if time is needed to allow the temperature of the sample to equilibrate in the magnet). The **Acquisition Pre-Delay Time** option allows such a delay to be set (in seconds). The waiting time is added to the recycle delay of the first scan of the data acquisition.

9.5 Dummy Shots

Pulses before the measurement can be made prior to the experiments (0-32000), in order to ensure that the first scan has the same history as all subsequent scans.

10 Maintenance

10.1 Cleaning

Before Cleaning

Disconnect the main cable from the unit before cleaning.

Cleaning the Main Unit

Use a clean damp cloth to wipe off any residue from the outside of the unit. Wipe off excess moisture immediately with a dry cloth.

For non water soluble marks, wipe using a cloth with a few drops of isopropyl alcohol.

Before Reconnecting the Power Supply

Wait until the unit is completely dry before reconnecting the power supply.



Figure 10.1: minispec mq-one SFC Analyzer in Pre-Heat Mode

Maintenance

11 Dismantling and Disposal

Following the end of its operational life, the unit can be returned to Bruker for safe disposal. If this is impractical, the unit should be disposed of safely as prescribed by local environmental regulations.



Installation, initial commissioning, retrofitting, repairs, adjustments or dismantling of the device must only be carried out by Bruker Service or personnel authorized by Bruker. Damage due to servicing that is not authorized by Bruker is not covered by your warranty.

11.1 Dismantling

Before starting dismantling:

- 1. Shut down the device and secure to prevent restarting.
- 2. Physically disconnect the power supply from the device; discharge stored residual energy.
- 3. Remove consumables, auxiliary materials and other processing materials and dispose of in accordance with the environmental regulations.
- 4. Clean assemblies and parts properly and dismantle in compliance with applicable local occupational safety and environmental protection regulations.

11.2 Disposal

If no return or disposal agreement has been made, send the dismantled components for recycling as prescribed by local environmental regulations.

- · Scrap metals.
- · Send plastic elements for recycling.
- Dispose of packaging material in accordance with the relevant applicable legal requirements and local regulations.
- · Sort and dispose of other components in accordance with their material composition.

NOTICE

Danger to the environment from incorrect handling of pollutants!

Incorrect handling of pollutants, particularly incorrect waste disposal, may cause serious damage to the environment.

- Always observe local environmental regulations regarding handling and disposal of pollutants.
- ▶ Take the appropriate actions immediately if pollutants escape accidentally into the environment. If in doubt, inform the responsible municipal authorities about the damage and ask about the appropriate actions to be taken.

Dismantling and Disposal

12 Diagnostics and Service: minispec.exe Software

The minispec.exe software is the standard software of the minispec mq-series analyzers. All details on that software are therefore located into the corresponding mq-series User's manual. Here a short summary of the usage of this software is presented only

In connection with the mq-one Analyzers, the minispec.exe software is used for diagnostic/service purposes only.

12.1 Configuration and Welcome Box

The configuration of the system (*i.e.* the connected minispec, the selected applications, the analyzer type, and the calibration permission) can be inspected and edited via the *Welcome Box*. The *Welcome Box* can also be user configured. Users can control whether or not this box will be opened on program start. This is done by selecting or deselecting the entry **Welcome Box** in the pull-down menu **View** (see also The View Menu). Deselecting the item **Display this Window on Startup** will also turn off the Welcome Box when the box appears on program start.

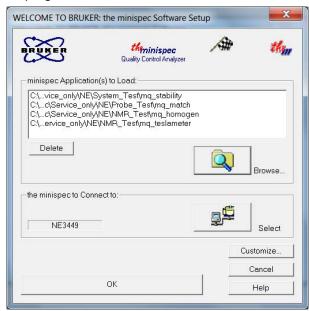


Figure 12.1: The Welcome Box

Several symbols, entries and buttons are displayed in the Welcome Box:

- Applications to be loaded (path and file name in the white field).
- · Serial number of the minispec to be connected to (here: NE3000).
- Type of analyzer (here: NMR Analyser).
- · The calibration permission is symbolized using a flag.



The 'wake-up' application can also be selected for future program start-up. When the user has finished with the selections, the 'OK' button is used to start the software.

Diagnostics and Service: minispec.exe Software

To change the configuration, press the **Setup** button. The configuration is protected by a simple log-in mechanism.

- First log-in: Press the Setup button. Enter and confirm a password. The password will be saved automatically and you will need it for every subsequent log-in. Handle the password carefully! Only users who have permission to make changes to calibrations and software configurations should have knowledge of the password. If password protection is not desired, simply click OK or <Enter> without entering a password when the password entry box appears and confirm this in the following box.
- Later log-in: Press the 'Setup' button and enter the password or click twice on **OK** if password protection is not used.

12.1.1 Selecting Applications and Connections

If you click **Setup** in the *Welcome Box* you will open the *configuration level* of the welcome dialogue. This password procedure is described in the section above. Up to 20 applications can be selected simultaneously for every analyzer type (except for the SFC-Analyzer where only one application is allowed) to be loaded at the startup. To add applications to the list use **Browse...** to access a file selector box or use **Delete** to remove applications from the list.

To choose another minispec, use the 'Select' button in the 'Select minispec to connect to' field.

12.1.2 Changing Analyzer Type and Calibration Permission

Use the **Customize** button in the *configuration level* (see *Selecting Applications and Connections* [68]) to open a dialog box. In this window the analyzer type and the calibration permission can be selected by checking the corresponding select box with a mouse click. Two options, RELAXATION TIME and the NMR analyzer, require a license number to operate. The number will be requested while connecting to the minispec (after you click the **OK** button in the *Welcome Box*) when one of these options is selected. If ordered with the system, this license number is issued on the first page of this booklet, labeled as the ExpSpel license number.

In general it is recommended not to alter the Analyzer Type, as the instrument settings are not automatically carried over when switching the analyzer types.

12.2 Menu Functions

The minispec.exe software provides many opportunities for data display, data saving, and measurement handling. This chapter describes all functions that are available when the software is configured as a *NMR-Analyzer*. All mq-one Analyzers are delivered configured as "QC" Analyzers and it is recommended not to change this.

When the minispec is used only for specialized applications (SFC, OIL) many of these functions are unnecessary. In this case, the number of menu options is reduced to simplify the interface and make the software easier to use when the configuration is adjusted to certain analyzer types. Commands whose functionality may be not reasonable in some contexts appear grayed or may no longer be visible.

The actions of the functions are described below.

12.2.1 The Bars

The minispec software menu structure and toolbars are designed within the framework of most standard Windows software to ensure intuitive handling (see the screen layout in the figure below). In the **Menu** Bar actions can be selected via pull-down menus. Icons are also used for commonly used actions and remain visible in the **Standard** Toolbar. Depending on the options selected, the most important commands for the execution and abortion of measurements may also be accessible through large icons on a **Measurement** Toolbar, which is usually positioned at the bottom of the screen below the signal window. In the **Result** Bar the numerical result(s) of the last measurement is displayed. The **Info** Toolbar contains easily selectable buttons pertaining to the instrument status and parameter display, as well as a list of loaded applications. Finally, the status of the measurement and connections are summarized in the **Status** Bar. The functionality of these items is described in the following sections in detail.

Adjustment of the bars (i.e. the possibility to move them) depends on the configuration of analyzer type you are working in. Repositioning of bars and windows is only allowed for the Relaxation Time and the NMR-Analyzer.

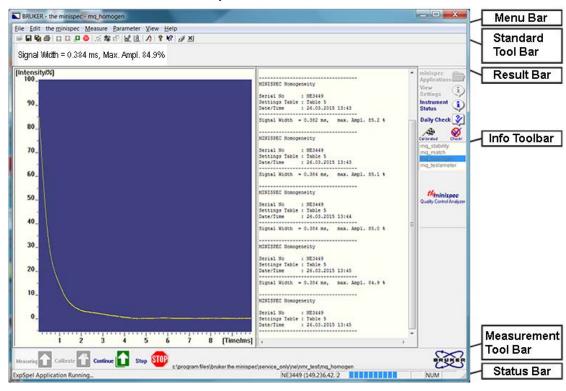
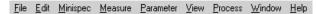


Figure 12.2: The Default View

The arrangement of the different bars supports an intuitive measurement handling.

12.2.2 The File Menu

The list of items in the **Menu** Bar depends on the active window. If the Signal Window is active, and an application is loaded, all entries are visible. The functions of the menu can be activated by a mouse click, or alternatively, using a keyboard shortcut (Alt + underlined letter).



By activating the **File** menu all commands necessary for file handling are available (see figure). Their use is in analogy to conventional Windows software, you can open, close, save or print the contents of the selected windows (or the whole application).

Diagnostics and Service: minispec.exe Software



Figure 12.3: The File Pull-Down Menu

The Open Command

Shortcuts: Standard Tool Bar:



Keys: CTRL+O

Use this command to open an existing document in a new window.

One can select either:

- A complete minispec application (filename extension .app) consisting of maximum four windows: an editor window with ASCII-text in ExpSpel programming language; the Signal Window with the measured signals; the Result Box; and in some cases a spreadsheet.
- Measured signals (filename extension .sig) and measured data Result Boxes (file name extension .mdt) separated from its minispec application.
- · Diagnostics files.

The Close Command

Use this command to close all windows in the active application or document.

If the focus is on one of the four views (windows) of a minispec application, the complete minispec application with all views will be closed.

Shortcut: Standard Tool Bar:



If you want to close all applications use:

Shortcut: Standard Tool Bar:



The Save command (Save As, Save Copy As)

Use the **Save** command to save the active document to its current name and directory. When you save a document for the first time, the minispec software displays the **Save Copy As** dialog box for input of a name. If you want to change the name and directory of an existing document before you save it, choose the **Save Copy As** command.

If you want to make a copy of an existing document, choose the **Save Copy As...** command.

Shortcuts: Standard Tool Bar:



Keys: CTRL+S

The Save Setup Command

The **Result** box displays results derived from the NMR data (after evaluation steps defined in the minispec application). Results are automatically saved as ASCII text at intervals (file extension: .mdt).

To set the parameters for the save procedure, select **Save Setup** from the result box file menu:

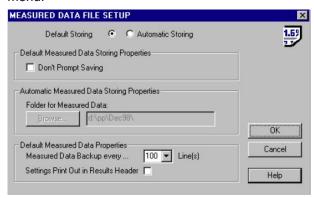


Figure 12.4: The Dialog Box for Data Saving Setup

Select **Default Storing** to backup every 100 result box lines of measured data to the file <application>.mdt in the current working directory.

When you attempt to exit the minispec application, the system will prompt whether the data should be saved, deleted or copied into another file.

Select **Don't Prompt Saving** to deactivate the prompt when saving, in which case the unsaved parts of the result box are then saved automatically. After reloading the minispec application, the results will be erased before the first new results are outputted to the Results box.

Select Automatic Storing for an automatic documentation of measured results.

The default path for saving is:

<current application directory>\<MMMJJ>\<ddhhmmss>.mdt

MMM: month
JJ: year
dd: day
hh: hour
mm: minute
ss: second

To modify the default path setting, select **Browse**... and define another folder. Default saving is every 100 lines and when leaving of the minispec application.

You can modify the default data saving behavior using Measured Data Backup every....

To include an output of the instrument and acquisition parameter settings, select **Settings Print Out in Results Header**. These settings are dependent on the minispec applications.

Diagnostics and Service: minispec.exe Software

The Print Command

Use this command to print a document. It opens a **Print** Dialog Box, where you may specify the range of pages to be printed, the number of copies, the destination printer, and other printer setup options.

Shortcuts: Standard Tool Bar:



Keys: CTRL+P

The Print Preview Command

Use this command to display the active document as it would appear when printed. The main window will be replaced with a print preview window in which one or two pages will be displayed in their print format. The **Print Preview** toolbar offers options to view either one or two pages at a time, movement back and forth through the document, zoom in and out of pages and to initiate a print job.

The Print Setup Command

Use this command to select a printer and a printer connection. This command presents a **Print Setup** dialog box where the printer and its connection are specified.

The 1, 2, 3, 4, 5 Commands

Use the numbers and filenames listed at the bottom of the File menu to open the last five documents you closed. Select the document you want to open.

The Exit Command

Use this command to end your minispec session. You can also use the **Close** command. The minispec software prompts you to save documents when unsaved changes exist.

Shortcuts: Headline:



Keys: ALT+F4

12.2.3 The minispec Menu

All commands concerning instrument settings are included in this menu item. The commands for the magnet heater calibration and the receiver tuning are only available for BRUKER service personnel and therefore are grayed with a normal software startup. The list of commands depends on the status of the instrument (see figure). If there is no application loaded, the list is enlarged by the commands **Connect** and **Disconnect**.

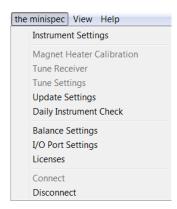


Figure 12.5: The minispec Pull-Down Menu

The Connect/Disconnect Command

Once the system requirements for TCP/IP have been fulfilled, a software link between the minispec software running on a PC, and the minispec must be initialized. To establish the PC to minispec connection, select **minispec Connect**. Alternatively you can select **Connect** in the **Welcome** Box.

Enter the minispec serial number when prompted by the Connection Dialog Box.

The minispec serial number must have the form 'NExxxx' for minispec mq-one systems.

The minispec serial number, which is the host name of the minispec, is used to identify the BRUKER minispec, controlled by the minispec software that is running on a PC in a TCP/IP network.

Use the command **Disconnect** from the menu to disconnect from the current minispec (e.g. prior to reconnecting to another minispec).

The Instrument Settings Command

The minispec instrument settings (see the figure below) are instrument dependent values such as the pulse lengths and the magnetic field at NMR resonance. Instrument settings differ from minispec to minispec, and must be tuned the first time a minispec is connected. You can use this command to change the settings of the instrument with manual input.

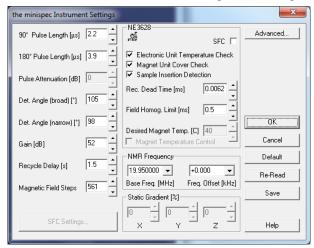


Figure 12.6: The minispec Settings Table



You can change the listed settings by manual input or with the Update Settings command. Greyed entries are disabled.

Diagnostics and Service: minispec.exe Software

Shortcut: Standard Tool Bar:



The settings that can be changed are shown in the figure above. If the **minispec Settings** are disabled on a connected minispec, customize your minispec software (through the Welcome Box) to access the calibration parameters.

The **Advanced** button in the settings table allows access to a list of instrument setting table names. The user may select the appropriate settings table to be used by the instrument, define custom names for the settings tables with the help of the **Customise** button (e.g. settings table name could be set to the probe name), and save the current entries under a new name.

SFC parameter (K, F, and O) factors are determined via the minispec Plus software only. Update Settings and Daily Check from minispec Plus will generate these SFC specific factors.

For special cases (like SFC automation systems) there exists a special license "mq-one SFC Automation License" to activate the calculation of the SFC specific factors in minispec.exe.

The Update Settings Command

A blue mark (validated) symbol on the right side of the **Info** Toolbar indicates a well checked minispec instrument.



An update of the instrument settings may be done periodically to check the instrument parameters, but is not necessary. An update may be necessary after the system has been relocated or the probe assembly has been changed. An instrument settings update is also recommended if the **Daily Check** fails.

The **Update Settings** routine starts from pre-adjusted settings (listed in the current instrument setting table). The Update Settings routine also allows the update of selective settings. For instrument optimization it is recommended using the **Update Settings** routine.

If the **Update Settings** menu stays disabled on a connected minispec, **customize** your minispec software (through the Welcome Box) to provide access to the calibration parameters.

The Daily Check Command

This option tests the instrument tuning but does not change the instrument settings. A quick check is recommended once a day (every 24 hours). A checkmark (checked) in the **Info** Toolbar signifies a well-checked minispec instrument. An un-calibrated minispec instrument is indicated by a yellow mark (Check!).



To run the Daily Check, use the corresponding toolbar button or select **Daily Check** from the menu. If one of the checks fails it indicates that an instrument setting is not optimized. Use the **Update Settings** command to perform an update.

Shortcut: Info Toolbar:



The Balance Settings Command

One can connect a scale by serial interface to the PC's communication port in order to electronically transfer sample weight information (weights are necessary for some absolute applications). To enter the port configuration dialog, close all minispec applications, then select **Balance** from the **Setup** menu. Access is limited to users who have permission to enter the minispec main menu or calibration. Select the balance type, then the port to connect the balance to. Select the port parameters according to the settings on the scale. To set the standard values, click **Default** before leaving the Settings Table. To leave the Settings Table unchanged, click **Cancel**. To re-load old settings from file after modifications, click **Re-Read**. To leave the Settings Table with the new values, click **OK**.

The I/O Port Settings Command

One can connect serial interface devices, such as balances, thermostats or sample changers, to the PC's communication port. To get the port configuration dialog, close all minispec applications, then select **I/O Port** from the **Setup** menu. Note: To get the minispec main menu, the R&D level or calibration permission must be given. Select the port parameters according to the settings on the connected device.

The Licenses Command

Some special applications, like the digital pulse attenuation and the pulse shaping need to be licensed. Use this menu to open the license number input box, which prompts the user to input the license number. After a successful license procedure, the menu entry is checked and grayed.

Have ready the minispec instrument's system number (see Status Bar) and contact BRUKER for information or license numbers.

See also

- Connecting the PC to the minispec for the First Time [▶ 39]
- minispec.exe Software: Wake-Up State [▶ 41]

12.2.4 The Measurement Menu

All commands concerning the execution of measurements are concentrated in this menu item (see the figure below). Since these commands are used frequently, quick select buttons are available in the Measurement Tool Bar and key short cuts exist to enhance accessibility.

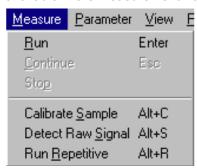


Figure 12.7: The Measurement Pull-Down Menu

Diagnostics and Service: minispec.exe Software

The Run, Stop and Continue Commands

The **Run** command starts a measurement. If the Sample Detector is set **ON** (see: Instrument Settings Command) the measurement will be executed automatically with the insertion of the sample.

Shortcuts: Standard Tool Bar:



Measurement Tool Bar:



Keys: ALT+M or ENTER

To interrupt a minispec measurement, use the **Stop** command.

Shortcuts: Standard Tool Bar:



Measurement Tool Bar:



The command **Continue** is used to leave an intermediate process in order to continue running the minispec application (e.g. during a waiting time, a data acquisition or a fit display).

Shortcuts: Standard Tool Bar:



Measurement Tool Bar:



Keys: ESC

The Calibrate Command

A typical minispec application detects NMR signals of the sample and then calculates the result from the NMR signal. In some cases, the result can be directly calculated from the measured signal (e.g. a relaxation time). In other cases the minispec applications may use a reference method and calibration line to determine a sample property (e.g. oil, water or fat content) from the NMR signal. As a consequence, the NMR signal must first be calibrated with respect to sample properties. Select **Calibrate Sample** from the **Measurement** menu.

Shortcuts: Standard Tool Bar:



Measurement Tool Bar:



Keys: ALT+C

Running a minispec sample calibration leads the user through several steps. In most cases some application specific values (see: The Application Parameter Table Command) need to be defined.

To calibrate a minispec application, proceed as follows:

- 1. Prepare at least 3 samples of known content for measurement.
- 2. Perform test measurements with each calibration sample to adjust the acquisition parameters from the **Acquisition Parameter Table** in the **Parameter** menu. Adjust the receiver gain to the sample with the strongest signal.
- 3. Save the parameters and leave the parameter table.
- 4. Run the sample calibration and follow the prompts.

A flag in the **Info** Toolbar indicates a calibrated minispec application.



An un-calibrated minispec application is labeled with the following flag:





Note: In case of mq-one Analyzers, the calibration is always done through the minispec Plus software.

Diagnostics and Service: minispec.exe Software

The Detect raw Signal Command

In some cases, for example to adjust the acquisition parameters, it might be helpful to detect the signal without data processing. This command was implemented to execute only the pulse sequence and acquisition without data processing or result output.

Shortcut: Keys: ALT+S

The Run Repetitive Command

With this command a measurement can be repeated several times at a regular interval.

Shortcut Keys: ALT+R

Select 'Repetitive Measurement Settings' from the Parameter menu to determine the waiting time in seconds before a repetitive minispec measurement, the delay between two successive repetitions, and the maximum number of repetitive measurements.

13 Contact

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Bruker BioSpin Hotlines

Contact our Bruker BioSpin service centers.

Bruker BioSpin provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the service center or hotline you wish to contact from our list available at:

http://www.bruker.com/service/information-communication/helpdesk/magnetic-resonance.html

Contact

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