

ITEM OPPORTUNITY SYNOPSIS

Scouting Number:	2024-098
Name of the item to be scouted:	Nuclear Magnetic Resonance (NMR) Spectrometer
State item to be used in:	North Carolina
Contract Manufacturer	
Please describe the item application/the end use of the item.	Commercially available benchtop nuclear magnetic resonance (NMR) spectrometer
Supplier Information:	
Type of Supplier Being Sought (select from the list below):	
Manufacturer	x
Contract Manufacturer	
Distributor	
Other (Please Specify)	
Reason for Scouting Submission (select from the list below)	
2nd Supplier	
Price	
Re-Shore	
Past supplier no longer available	
New Product Startup	
BABA	x
Other (Please Specify)	
Summary of Technical Specifications and Performance Requirements:	
Describe the manufacturing processes (elaborate to provide as much detail as possible)	All standard manufacturing processes required to produce a nuclear magnetic resonance (NMR) spectrometer scientific instrument capable of autonomous NMR measurement, data processing, and data extraction. Manufacturing capabilities may include but are not limited to: injection molding, metal casting, electronic manufacture and assembly, precise set up of sensitive analytical equipment, software development accompanying the extraction of NMR data, and IT construction and development for use of the instrument and extraction of data.
Provide dimensions / size / tolerances / performance specifications of the item	NMR must be able to fit compactly on a standard-sized scientific benchtop/workspace. Please see attached product brochure for commercial specifications. Please see attached specifications document for required salient characteristics.
List required materials needed to make the product, including materials of product components, if applicable	Product is a complex scientific instrument intended for the identification, determination and/ or confirmation of chemical structures, from small and simple molecules to larger and more complex species, including possibilities of monitoring reactions and kinetic. The instrument is controlled via software installed on a computer. Many materials and processes would be required to replicate the instrument, please see attached product brochure for more information and image of equipment.
Are there applicable certification requirements?	
Yes	x
No	
Please explain:	All certifications for laboratory equipment to be utilized in the United States are applicable.
Are there any applicable regulations that apply to the production of this item?	
Yes	x
No	
Please explain:	All regulations for laboratory equipment to be utilized in the United States are applicable.
Are there any other standards / requirements?	
Yes	x
No	
Please explain:	All standards and requirements for laboratory equipment to be utilized in the United States are applicable.
Additional Comments:	
Additional technical comments:	Must be commercially available and fit the salient characteristics

Volume and Pricing:	
Estimated Potential Business Volume (i.e. #units per day, month, year):	This is a one time solicitation for a commercially available NMR spectrometer, which must fit the salient characteristics listed on the attached specifications document.
Estimated Target Price/Unit Cost Information:	US EPA has been quoted \$149,568.26 for the supply, initial setup, and 12 month warranty of one (1) Fourier 80 NMR spectrometer manufactured and sold by the Bruker Corporation.
Delivery Requirements:	
When is it needed by? (Immediate, 30 days, 6 months, etc.)	Need is immediate.
Describe packaging requirements (i.e. individually/group packaging, etc.)	N/a; packaged according to industry standards.
Where will this item be shipped?	Research Triangle Park, NC
Additional Comments:	
Is there other information you would like to include?	Vendor/company must be registered or will register in SAM.gov (https://sam.gov/content/home). This inquiry does not guarantee award of contract.

Fourier 80

- Spectrometer
User Manual
Version 003



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1 Introduction

This document describes the basic operation of the Bruker NMR spectrometer Fourier 80. In this context, the acronym *NMR* means *Nuclear Magnetic Resonance*. The spectrometer is controlled almost entirely via user software, which includes defined workflows for an easy and fast experiment setup.



Based on its various applications, some fundamental NMR expertise as well as special knowledge is required which could not be detailed in this manual.

1.1 Intended Use

The Bruker Fourier 80 is a benchtop system developed as a Fourier-Transform Nuclear Magnetic Resonance (FT-NMR) spectrometer based on a cryogen-free permanent magnet operating at 80 MHz ^1H resonance frequency. As an FT-NMR instrument, the Fourier is intended to be used for the identification, determination and/ or confirmation of chemical structures, from small and simple molecules to larger and more complex species, including possibilities of monitoring reactions and kinetics.

The device has been designed and constructed solely for the intended use described here. Intended use also includes compliance with all specifications within this manual.

The device is not intended for the use of:

- Radioactive samples
- Biohazard-labeled samples

For more information contact your local Bruker representative.

Any use which exceeds or differs from the intended use shall be considered improper use. No claims of any kind for damage will be entertained if such claims result from improper use.

1.2 Policy Statement

It is Bruker's policy 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. Field Service Engineers are advised to check regularly with Bruker for updated information.

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

1.3 Limitation of Liability

All specifications and instructions in this manual have been compiled taking into account applicable standards and regulations, the current state of technology and the experience and insights we have gained over the years.

The manufacturer accepts no liability for damage due to:

- Failure to observe this manual.
- Improper use.
- Deployment of untrained personnel.
- Unauthorized modifications.
- Use of inadmissible spare parts.

The actual scope of supply may differ from the explanations and depictions in this manual in the case of special designs, take-up of additional ordering options, or as a result of the latest technical modifications.

The undertakings agreed in the supply contract, as well as the manufacturer's Terms and Conditions and Terms of Delivery, and the legal regulations applicable at the time of the conclusion of the contract shall apply.

1.4 Warranty Terms

The warranty terms are included in the manufacturer's Terms and Conditions.

1.5 Customer Service

Our customer service division is available to provide more information about our product. See the chapter Contact for contact information.

In addition, our employees are always interested in acquiring new information and experience gained from practical application; such information and experience may help improve our products. Feedback from our customers is highly appreciated.

1.6 Product Safety and Electromagnetic Compatibility

The device complies with the standard

- IEC 61010-1 and with UL 61010-1 / CSA C22.2 No. 61010-1-04 Safety Requirements for Electrical Equipment.
- IEC 61326-1 for Electromagnetic Compatibility (EMC)

2 Safety

This section provides an overview of all the main safety aspects involved in ensuring optimal personnel protection, as well as safe and smooth operation.

Non-compliance with the action guidelines and safety instructions contained in this manual may result in serious hazards.

2.1 General

There are no user-serviceable parts inside the Fourier spectrometer. Refer servicing to qualified service personnel.

2.2 Symbols and Conventions

Safety instructions in this manual have a clear structure based on the ANSI Z535.6 standard, listing the danger, consequences of non-compliance and possible solutions. Therefore, they are also conform with DIN EN 82079-1.

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 that, if not avoided, will result in death or serious injury.



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



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



NOTICE is used to address practices not related to personal injury.

2.3 System Owner's Responsibility

System Owner

The term *system owner* refers to the person who operates the device for trade or commercial purposes, or who surrenders the device to a third party for use/application, and who bears the legal product liability for protecting the user, the personnel or third parties during the operation.

System Owner's Obligations

The device is used in the industrial sector, universities and research laboratories. The system owner of the device must therefore comply with statutory occupational safety requirements.

In addition to the safety instructions in this manual, the safety, accident prevention and environmental protection regulations governing the operating area of the device must be observed.

In this regard, the following requirements should be particularly observed:

- The system owner must obtain information about the applicable occupational safety regulations, and - in the context of risk assessment - must determine any additional dangers resulting from the specific working conditions at the usage location of the device. The system owner must then implement this information in a set of operating instructions governing operation of the device.
- During the complete operating time of the device, the system owner must assess whether the operating instructions issued comply with the current status of regulations and must update the operating instructions if necessary.
- The system owner must clearly lay down and specify responsibilities with respect to installation, operation, troubleshooting, maintenance and cleaning.
- The system owner must ensure that all personnel dealing with the device have read and understood this manual. In addition, the system owner must provide personnel with training and hazard information at regular intervals.
- The system owner must provide the personnel with the necessary protective equipment.
- The system owner must warrant that the device is operated by trained and authorized personnel as well as all other work, such as transportation, mounting, start-up, the installation, maintenance, cleaning, service, repair and shutdown, that is carried out on the device.
- All personnel who work with, or in the close proximity of the device, need to be informed of all safety issues and emergency procedures as outlined in this user manual.
- The system owner must document the information about all safety issues and emergency procedures in a laboratory SOP (Standard Operating Procedure). Routine briefings and briefings for new personnel must take place.
- The system owner must ensure that new personnel are supervised by experienced personnel. It is highly recommended to implement a company training program for new personnel on all aspects of product safety and operation.
- The system owner must ensure that personnel are regularly informed of the potential hazards within the laboratory. This is all personnel that work in the area, but in particular laboratory personnel and external personnel such as cleaning and service personnel.
- The system owner is responsible for taking measures to avoid inherent risks in the handling of dangerous substances, preventing industrial disease, and providing medical first aid in emergencies.
- The system owner is responsible for providing facilities according to the local regulations for the prevention of industrial accidents and generally accepted safety regulations according to the rules of occupational medicine.
- All substances needed for operating and cleaning the device samples, solvents, cleaning agents, gases, etc. have to be handled with care and disposed of appropriately. All hints and warnings on storage containers must be read and adhered to.
- The system owner must ensure that the work area is sufficiently illuminated to avoid reading errors and faulty operation.
- The system owner must ensure that the laboratory is equipped with an oxygen warning device, in case the device is operated with e.g. nitrogen or helium.

Furthermore, the system owner is responsible for ensuring that the device is always in a technically faultless condition. Therefore, the following applies:

- The system owner must ensure that the maintenance intervals described in this manual are observed.
- The system owner must ensure that all (electrical, mechanical, etc.) safety devices are regularly checked to ensure full safety functionality and completeness.

2.4 Personnel Requirements



Only trained Bruker personnel are allowed to mount, retrofit, repair, adjust and dismantle the unit!

2.4.1 Qualifications

This manual specifies the personnel qualifications required for the different areas of work, listed below:

Laboratory Personnel

Laboratory personnel are professionals, technicians, and assistants staffing a research or industrial facility where specimens are synthesized, tested, or evaluated and the results of such measurements are recorded. Laboratory personnel are able to carry out assigned work and to recognize and prevent possible dangers self-reliant due to their professional training, knowledge and experience as well as profound knowledge of applicable regulations.

The workforce must only consist of persons who can be expected to carry out their work reliably. Persons with impaired reactions due to, for example, the consumption of drugs, alcohol, or medication are prohibited from carrying out work on the device.

When selecting personnel, the age-related and occupation-related regulations governing the usage location must be observed.

2.4.2 Unauthorized Persons

WARNING

Risk to life for unauthorized personnel due to hazards in the danger and work zone!



Unauthorized personnel who do not meet the requirements described in this manual will not be familiar with the dangers in the work zone. Therefore, unauthorized persons face the risk of serious injury or death.

- ▶ Unauthorized persons must be kept away from the danger and work zone.
- ▶ If in doubt, address the persons in question and ask them to leave the danger and work zone.
- ▶ Cease work while unauthorized persons are in the danger and work zone.

2.4.3 Instruction

Personnel must receive regular instruction from the owner. The instruction must be documented to facilitate improved verification.

The name of the person who received the instruction, the name of the instructor, the type of instruction and the date must be documented and signed.

2.5 Basic Dangers

The following section specifies residual risks which may result from using the device and have been established by means of a risk assessment.

In order to minimize health hazards and avoid dangerous situations, follow the safety instructions specified here as well as in the following chapters of this manual.

2.5.1 General Workplace Dangers

⚠ 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.

2.5.2 Magnetic Fields

In order to ensure user's health and safety the system owner needs to control or rather authorize access to the NMR-system in accordance with national and local regulations.

From an EMF-perspective, the magnet exhibits a very good shielding with a minimal magnetic stray field of $< 0.2 \text{ mT}$ (2 Gauss) outside the housing of the instrument. Therefore, the "group of people at particular risk" (persons with active or passive implants, people wearing medical devices or pregnant women) are at neglectable risk when working in the vicinity of the instrument. Nevertheless, all persons working with the system should be informed about the existence of the magnetic field.

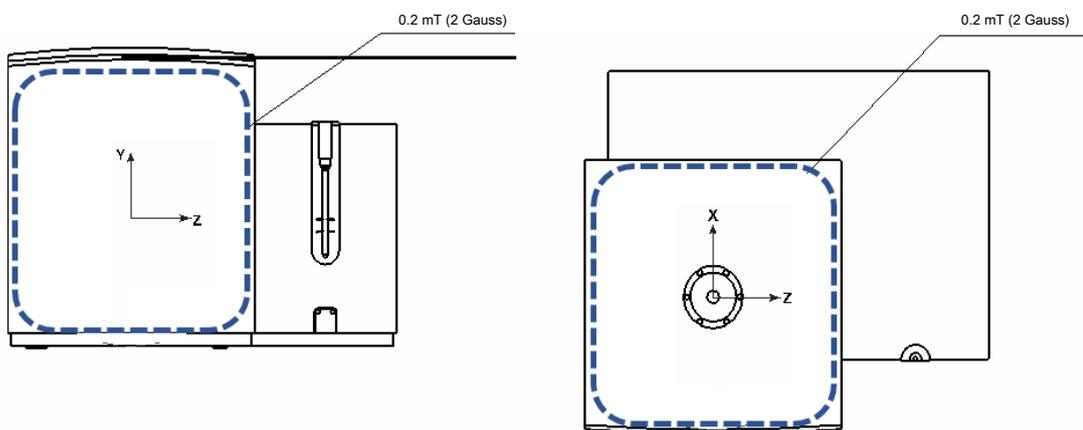


Figure 2.1: Stray Field Line Front and Top Views

⚠ CAUTION**Risk of injury and/or property damage due to the static magnet field!**

The significant hazard potential within a static magnet field comes from metallic and ferromagnetic objects. They are attracted and can damage the spectrometer, if they attain the magnet bore. Among other things, examples of this are scissors, pins, coins and (infusion) needles.



- ▶ Do not carry any objects which could affect the system's functionality (e.g. image quality of scans).
- ▶ Due to the magnetic field, electronic data mediums could be deleted/destroyed and sensitive objects could be damaged.
- ▶ Before entering the access-controlled area or the stray field, drop all metallic, ferromagnetic and sensitive objects (e.g. scissors, needles, credit cards, clocks).
- ▶ Make sure that all objects brought into the stray field/access-controlled area are neither metallic nor sensitive, and will not cause any problems during the system's operation.

2.5.3 Non-ionizing Radiation

⚠ CAUTION**Risk of injury from non-ionizing radiation.**

Due to missing knowledge about the usage of NMR systems and non-ionizing radiation that originates from the system can cause personal injury and damage its environment.



- ▶ Only use this spectrometer, if the user is familiar with the usage of NMR devices/instruments.
- ▶ Observe all national and local health and safety regulations when working in areas with non-ionizing radiation.

2.5.4 Electrical Safety

⚠ WARNING**Risk to life from electrical shock**

A life-threatening shock may result when the housing is open during operation.



- ▶ Only qualified personnel should open the housing.
- ▶ Disconnect the device from the electrical power supply before opening the device. Use a voltmeter to verify that the device is not under power!
- ▶ Be sure that the power supply cannot be reconnected without notice.

2.5.5 Hot Materials



CAUTION

Risk of injury due to hot materials!

Some components, accessories (e.g. temperature unit) and/or substances become very hot during operation and, therefore, can cause burns (also irreversible).

- ▶ Do not touch these components and/or substances during operation!
- ▶ Handle such components, accessories or substances with utmost caution.

2.5.6 Fragile Materials



CAUTION

Risk of injury or material damage from broken glass/sample tubes

Improper handling of the sample tubes may result in material damage and personal injury caused by glass fragments.

- ▶ Handle the sample tubes carefully, because they are fragile and can easily break.
- ▶ Insert and remove the sample tubes with utmost caution.

2.5.7 Hazardous Samples

Besides the hazard described above, there might be hazard caused by the sample (material).



WARNING

Risk of injury or death due to hazardous samples

Infectious, radioactive, corrosive as well as other hazardous sample material can cause health injury (also irreversible) or can result in death.

- ▶ Observe standards and regulations valid for your laboratory.
- ▶ Take appropriate protective and disinfection measure (e.g. wearing protective clothing, mask).

2.6 Environmental Protection

NOTICE

Potential environmental damage 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.

Waste disposal

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

2.7 Emergency Shutoff

The mains switch on the back of the Fourier 80 consoles serve as an EMERGENCY OFF. If the main switch is not easily accessible due to the placing of the instrument, please pull the power cable from the power plug in case of an emergency.

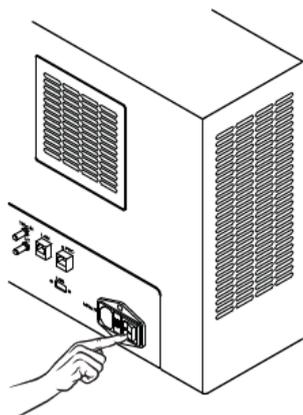


Figure 2.2: Location of the Emergency Shutoff Switch

2.8 Signs and Labels

The following labels and safety signs are affixed to the system and must be kept legible at all times. Replace worn or damaged labels and safety signs immediately.

Label / Safety Sign	Definition
	<p>This safety sign is located on the rear side and indicates that you need to disconnect the system from main supply before opening the housing/cover.</p> <ul style="list-style-type: none"> • Only authorized personnel may open the housing/cover for maintenance or repair! • Non-observance can cause personal injury and/or property damage!

3 Packaging, Storage and Transportation



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 warranty.

3.1 Symbols on the Packaging

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

Top		The arrow tips on the sign mark the top of the package. They must always point upwards; otherwise the content may be damaged.
Fragile		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 From Moisture		Protect packages from moisture. Keep dry at all times.
Attach Here		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		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.

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 Discharge		The packaging contains components which are sensitive to an electrostatic discharge. Only allow packaging to be opened by trained personnel. Establish potential equalization before opening.
Protect from Heat		Protect packages against heat and direct sunlight.
Protect from Radioactive Sources		Protect packages against 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 apparent external transport damage:

- Do not accept the delivery or accept only under reservation.
- Note the extent of the damage on the transport documentation or the shipper's delivery note.
- Initiate complaint procedure and document the condition of the transport damage with high quality photos (sharp, unshaken, everything legible).



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. The components should stay packed until just prior to installation.

Handling Packaging Materials

Keep the original container and packing assembly, at least as long as the warranty is valid, in case the unit has to be returned to the factory. When the packaging material is no longer needed dispose of it in accordance with the relevant applicable legal requirements and local regulations.

3.4 Storage & Transportation

Climatic Conditions for Storage & Transportation

- Store the packages according to the climatic conditions defined in IEC 60721-3-1, classification level 1K21.
- For the transportation, it is recommended to comply with the climatic conditions defined in IEC 60721-3-2, classification level 2K11.



Under certain circumstances, storage instructions may be affixed to packages that extend the requirements specified here. Comply with these accordingly.

4 Design and Function

This chapter describes the function of the Fourier 80 spectrometer and its components. The spectrometer can be equipped with optional accessories, which enlarge its range of functions but also making it look slightly different.

4.1 Overview

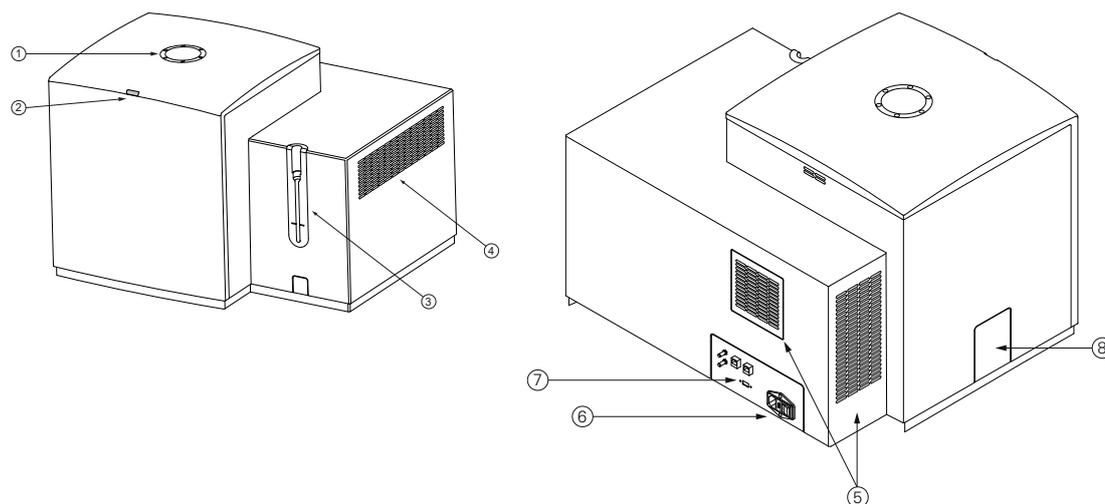


Figure 4.1: Overview Front and Back

1	Sample opening/slot	5	Ventilation grids
2	Status LED	6	Mains ON/OFF switch
3	Sample positioning gauge	7	Ports for communication and supply
4	Ventilation grid	8	Port for optional accessories.

4.2 Functional Description

The Fourier 80 is an analytical benchtop system for general NMR measurements developed with the highest standards of usability and operating comfort.

It is intended to be used for analyzing liquid samples. The system consists of a single housing containing the electronic unit and a magnet, a computer and the user software (TopSpin and GoScan). The system is delivered with an USB stick with an easy to install backup of the operating system, the TopSpin and GoScan user software including all default settings, and various user manuals. Due to its easy handling this spectrometer is well suited for entry level users and daily routine tasks.

The GoScan user software consists of an easy to use acquisition Graphical User Interface (GUI), with TopSpin (4.0.8 or higher) running in the background.

4.2.1 PC Hardware

The Fourier 80 spectrometer is delivered as default with the following workstation ¹:

- HP MS-Windows PC Mini
- HP monitor with touchscreen (23")
- At least 1920 x 1080 at 60 Hz
- At least Windows 10, Intel® Core™ i3 Processor, 16 GB SDRAM; 256 GB SSD

4.3 Connections

4.3.1 Back Panel

The ports for communication and supply are located on the system's back panel.



For safety reasons, all system connections need to be easily accessible at any time! In addition, it also must be possible to quickly disconnect the system from the mains supply in case of an emergency.

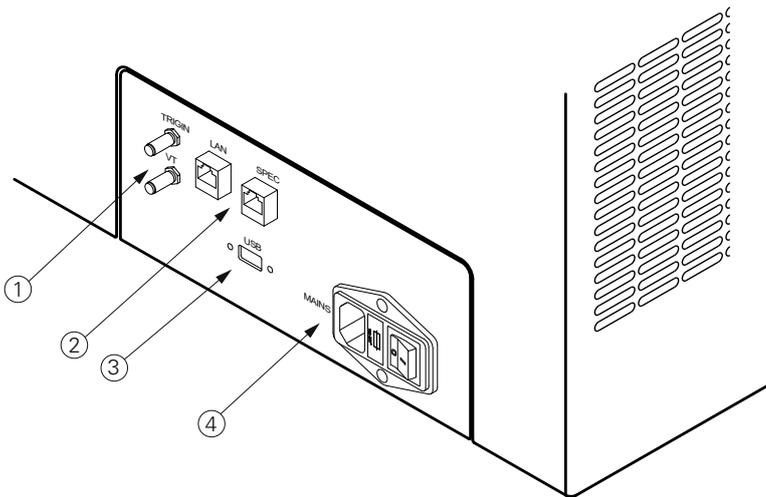


Figure 4.2: Connections on the Back Side

1	TRIGIN: Customer cutting point (TTL 5V signal in / signal out) VT: Port for Bruker to monitor temperatures during servicing.
2	SPEC: Communication interface to PC (certified Ethernet cabled supplied in the accessory kit). LAN: Communication interface to network.
3	USB port. Communication interface for diagnostics and maintenance.
4	MAINS: Line-in unit containing ON/OFF-switch, fuse box and safety plug for power supply.

¹ Specifications may change without further notice.

4.3.2 Side Panel

The spectrometer is equipped with an additional port, which is located on the left side panel. This port can be replaced by a connector for future optional accessories.

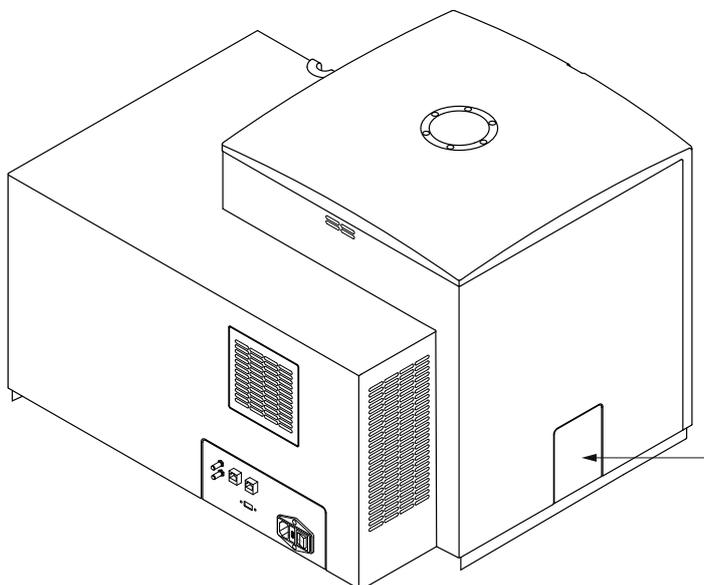


Figure 4.3: Optional Accessories Port

4.4 Status LED

The spectrometer has a status LED located on the front, which can have the following listed color states.

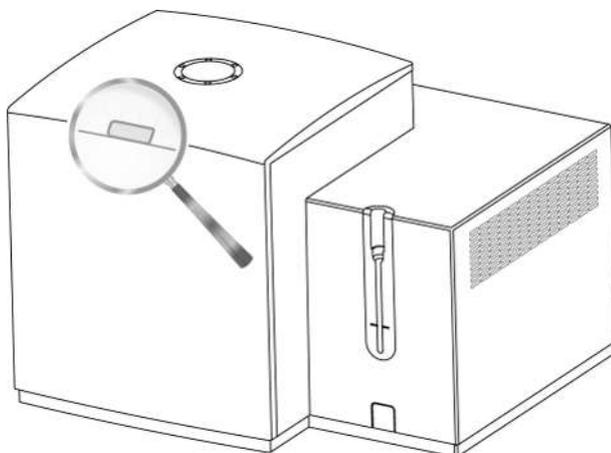


Figure 4.4: Location of the Status LED on the Fourier 80

Color	Status Description
Blue	Ready for operation.
Orange	Device is starting or not yet stable enough for measurements.
Red	Error.
None	Off.

Please note that on the date of publication of this manual, the LED is without function. This will be changed with one of the upcoming firmware releases. Uploading of the new firmware will be made possible in the field by a TopSpin update.

The GoScan user software also contains a status indicator.

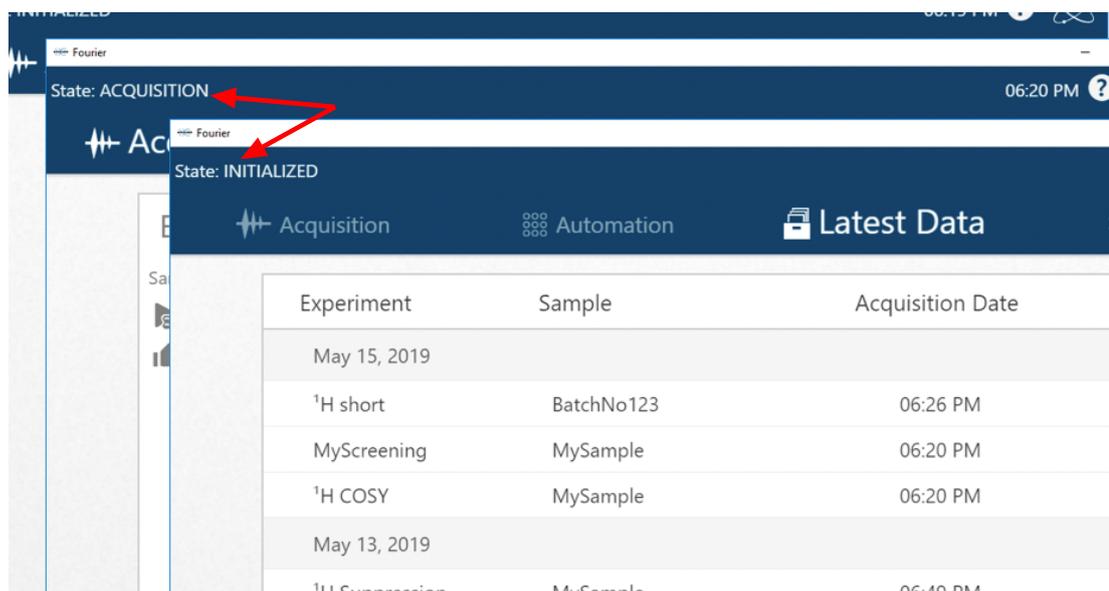


Figure 4.5: Status Indicator in GoScan

In TopSpin “Spectrometer running” appears in the status bar and during experiments there is an acquisition status indicator if this is selected in the preferences. Refer to the online help in TopSpin for more information.

5 Installation

Unpacking and initial installation can be done by the customer. It will be done by professionals authorized by Bruker if this option was included in the contract. The installation procedure needs to be documented.

5.1 Site Planning

The System Owner must provide an installation site that meets the site requirements described in this section.

General requirements for the installation of the device:

- Use only indoors.
- Do not operate in humid environments.
- Do not expose to direct sunlight.
- Do not operate in chemically aggressive environments.

NMR instruments are sensitive to mechanical vibrations, external magnetic fields and room temperature changes.

Vibrations

The Fourier 80 must be placed on a stable bench or table (see [Technical Data \[57\]](#) for the weight of the unit) and no other equipment which produces vibrations should be placed on the same table. Typically, vibrations can be seen as random distortions in the base of larger resonance lines. The Shim Sample can be used to detect vibration artifacts.

Magnetic Stray Fields

WARNING



This is a class A product.

In a domestic environment this product may cause radio interference in which case the user may be required to take adequate measures.

- ▶ Avoid installation in the vicinity of large electromagnetic fields such as overhead lines of a railway line.

The Fourier 80 produces only a very small magnetic stray field outside of its housing (< 2 G or 0.2 mT). Therefore, it has no considerable influence on magnetizable material in the vicinity of the system. But magnetic fields from the outside can influence the shim and lock of the Fourier 80. Avoid bringing magnetic tools or equipment close to the system. Also avoid placing the system close to large moving metallic structures like elevators or cranes.

An additional source of magnetic fields can be power lines close to the system. Their effect can be seen as modulations of high magnitude resonance lines. The modulations are symmetrical to each resonance line and have a frequency offset which exactly corresponds to the frequency of the external distortion (e.g., 50 Hz/60 Hz). It can help to change the routing of power cables close to the Fourier 80. If the distortion results from, e.g., a nearby external high-voltage line, it can be drastically reduced by turning the Fourier 80 into a different orientation. This is because only magnetic field components parallel to the field direction of the Fourier's magnet have an influence on the NMR spectra.

Temperature Changes

Permanent magnets have a high dependency of their field strength on temperature. To avoid drifts of the magnetic field due to temperature changes of the environment, the Fourier 80 uses two interleaved insulated boxes and an active control to keep the magnet at a very stable temperature. In order to reach the specified stability, the room temperature must not be outside of the range from 18 °C to 28 °C. Furthermore, the temperature changes over time should be less than +/- 1.5 °C per day. Very fast fluctuations within several minutes as well as very slow fluctuations over the day are less critical because they are compensated by the high specific heat of the magnet and the temperature regulation of the system.

Electrical Power Requirements

The Fourier 80 needs about 200 W of electrical power from a standard power outlet. Its internal wide-range power supply accepts 110-240 V, 50-60 Hz AC. In case of instabilities of the provision of electricity, an uninterruptable power supply UPS is recommended in order to have a steady temperature regulation of the Fourier 80 magnet.

General Workplace Requirements

In order to ensure a proper and safe handling the following listed requirements need to be observed when placing the system on its workplace.

- The system needs to be placed on a stable, horizontal and flat surface designed to take the system's weight (see [Technical Data \[p 57\]](#)).
- The system needs to be placed at a minimum distance of 5 cm from surrounding walls on all sides. Thereby, make sure that cables and hoses are not kinked.
- All connections always need to be easily accessible.
- The system should be placed in such a manner, that the sample opening on the system's top side can be accessed conveniently.
- The system should be installed in a well-ventilated room, or a ventilation system should be used.

Observe all the specifications of the existing laboratory standards and occupational safety regulations when arranging the workplace as well as during daily work. If you have any questions, contact your safety officer.



For questions concerning ambient conditions, electrical interferences and power supply refer to the section [Specifications \[p 58\]](#).

5.2 Benchtop Installation

This section will describe the installation of the standard configuration. The installation may vary depending on optional components and/or accessories:

Standard components:

Item	Description	Part Number	Quantity
Fourier 80 Standard Unit	Spectrometer with electronic unit, magnet and user software package.	H168135	1
Fourier 80 External Cable Set	Power supply cable. Ethernet cable for system integration.	H168174	2
USB Stick	Fourier 80 Software Installer Fourier 80 User Manual	H176416	1
Fourier 80 Accessory Kit	Accessory Kit with various tools, sample holder, etc.	H176415	1
Fourier 80 User Manual	Printed Fourier 80 User Manual	H172348	1

Table 5.1: Fourier 80 Standard Benchtop System Components

Optional components

- Lift truck.

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.

Spectrometer placement

- The spectrometer is delivered in a wooden box. Please check the shock and tilt indicator on the outside of the shipping box. Both must not be triggered. Remove the top of the shipping box. Take out all of the boxes and the cushioning. One box contains the tools to install the system. Use the Torx-key to remove the screws at the bottom of two of the sidewalls and remove the sidewalls.

If there are visible signs of damage or missing components or if the shock or tilt indicator is triggered, contact the Bruker Service Helpdesk.

Installation

- Use a lift truck to pick up the pallet and raise it to the table height using the foot pump.



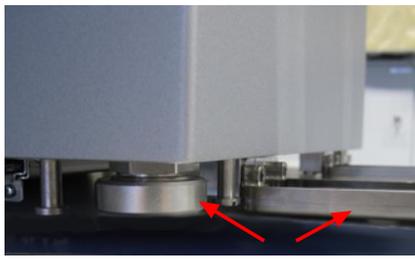
Note that some lift trucks have a hydraulic system valve, which prevents oil from leaking the lift truck during transportation

- Open the valve before operating the platform lift.

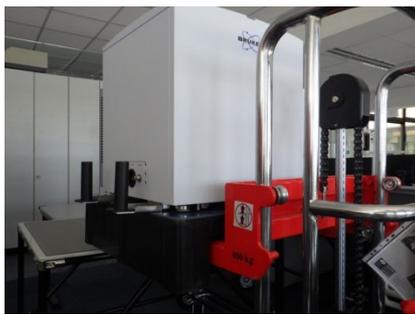


- To position the lift truck precisely, use the foot pump to move the lift truck's fork upward and turn the red hand wheel slowly to move the fork downwards.

- Remove the fixing screws on the pallet.



Before the spectrometer is moved, it should be checked that the feet are turned up!! They should not come in contact with the pallet. If necessary, turn the 4 unit feet upwards using the supplied open-end wrench, until the unit rests on the two transport rails, which are located on the left and right of the bottom of the device.



Spectrometer with pallet on the pallet truck (P/N 1822480).



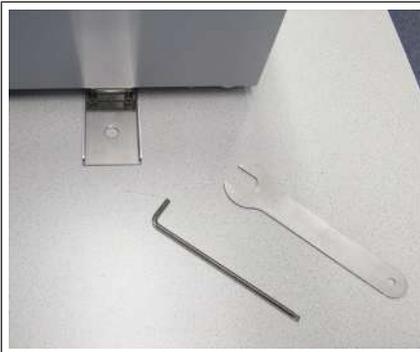
Move the pallet to the edge of the table and set it flush with the edge of the table and pallet edge, activate the parking brake of the lift truck.



Carefully slide the spectrometer onto the table using the handles located on the bottom of the spectrometer.



Unscrew the handles using an Allen key and remove them from the spectrometer.



Tools:

1 x Allen key.

1 x combination wrench P/N H138346.



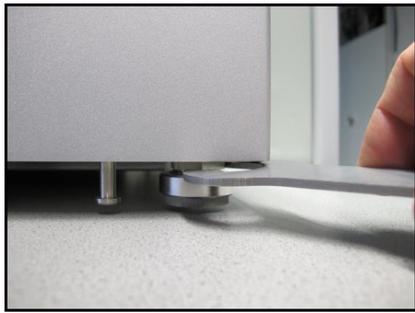
Transport plates.



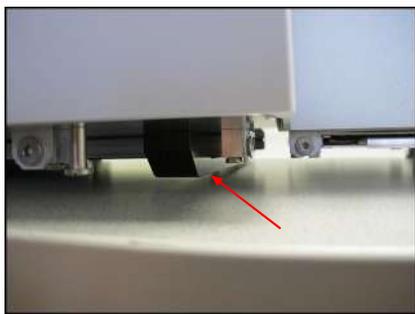
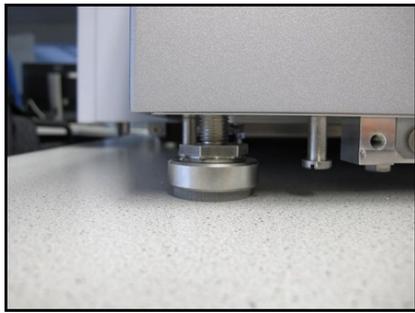
Remove the transport plates using the Allen key.



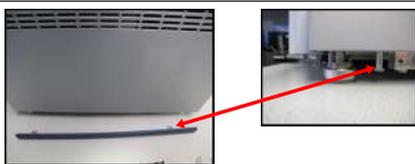
The device can now be moved to the desired location.



Turn the adjustable feet counterclockwise downwards, using an open-end wrench, until the spectrometer rests level and firmly on the stand.



Slide the transport rails out of contact with the table.



Clamp the decorative trim on the spectrometer.



5.3 Connecting to a PC

Connect the network cable to the PC and the Ethernet port labeled SPEC located on the rear side of the spectrometer. On the PC, configure the network interface so that it obtains the configuration from a DHCP server.

For details concerning the spectrometer interfaces, ports and/or connectors see section [Connections \[20\]](#).

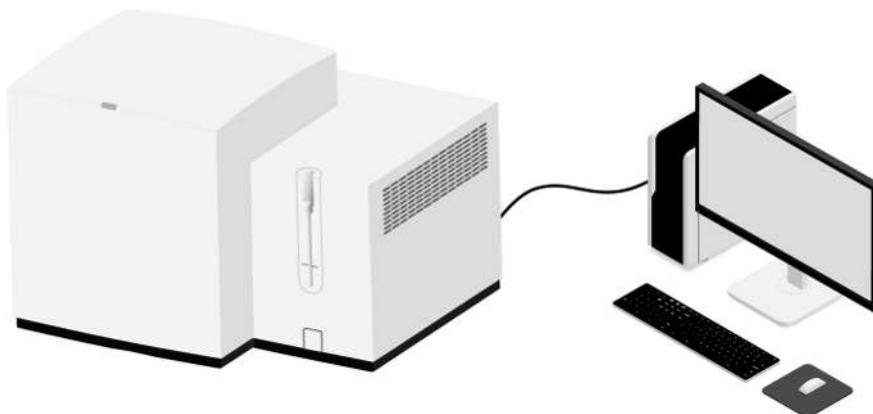


Figure 5.1: Scheme — Single PC

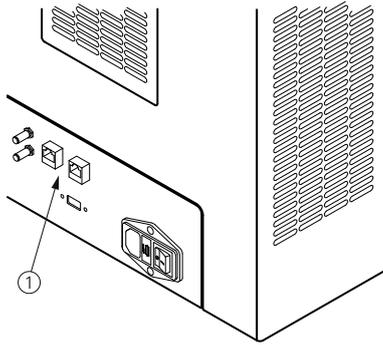


Figure 5.2: Spectrometer Ethernet Port

5.4 Connecting to the Mains Supply

The spectrometer's power connector is located on the rear side of the device.

- Connect the spectrometer to the mains supply using the delivered power supply cable.



For detailed specifications for the power supply see [Specifications \[58\]](#).

6 Operation

The Fourier 80 spectrometer is operated exclusively through the user software. Components are selected and controlled using the corresponding software functions. This chapter describes how to start and setup the Fourier 80.

- Once the system is placed on a table (see [Benchtop Installation \[25\]](#)) it can be switched on. The PC or Laptop can be connected to the Fourier 80 before starting the system or at a later time.

6.1 Starting the Fourier 80

The power switch is located on the back panel of the spectrometer. Press the switch. The spectrometer will take some time to boot and to stabilize the temperature of the magnet. It is Ready to use when the status LED on the front lights blue permanently.

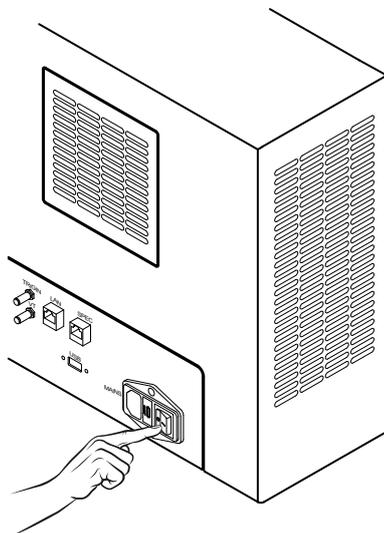


Figure 6.1: Location of the Power Switch

The system boots up autonomously because the firmware is stored on the system itself. It also starts the temperature control of the magnet and re-loads the factory shim. The latter is important because the shim currents also contribute to the temperature of the magnet.

If the system was switched off for a longer time, i.e., more than some hours, the stabilization of the magnet temperature may take several hours. It is best to wait for the system to stabilize overnight. The LED on the front will indicate that the Fourier 80 is ready to be used by turning from orange to blue.

In case the PC is not already connected to the Fourier 80, it should be done now. The PC comes with a pre-installation of TopSpin and all relevant parameters have already been determined and stored during the factory configuration and endtest.

After starting the Fourier 80, open TopSpin and check if TopSpin connects to the Fourier 80. This can be seen as a status notification "Spectrometer running" in the Acquisition Status Bar at the bottom of the TopSpin main window.

If TopSpin cannot find a spectrometer, it shows a notification in a pop-up window that informs you that TopSpin is not connected to a spectrometer hardware and, therefore, configures as a data station. In this case, check the LAN or WLAN connection from the PC to the Fourier 80 and the settings of the respective Ethernet adapters of the PC. If the problem is resolved, restart TopSpin.

Leave the Fourier 80 on all the time to maintain temperature stability.

6.2 Setting Up the Fourier 80

The Fourier 80 is pre-configured and does a lot of things autonomously like heating up the magnet and re-loading a factory shim file. The relevant files describing the hardware properties were generated at the factory and the configuration was performed. The spectrometer frequency was also set to the correct value and the parameter sets were pre-installed. In addition, the shim file from the set-up during endtest was stored and the table defining the pulse power for several pre-defined pulses (prosol) was set up.

In addition, some actions must be taken by the customer to finalize the set-up of the system. This requires putting in the shim sample which is delivered with the system and starting the set-up procedure by typing **bringup** into the TopSpin command line.

6.2.1 Sample Insertion

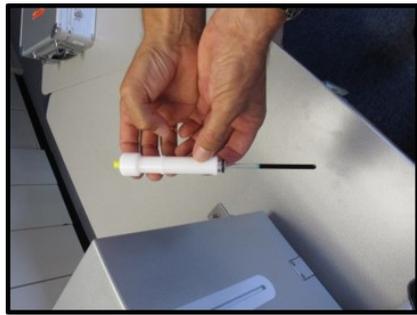
This section describes how to insert a sample into the Fourier 80 for measurements.



Sample and Sample Holder.



Insert the sample into the sample holder from above.

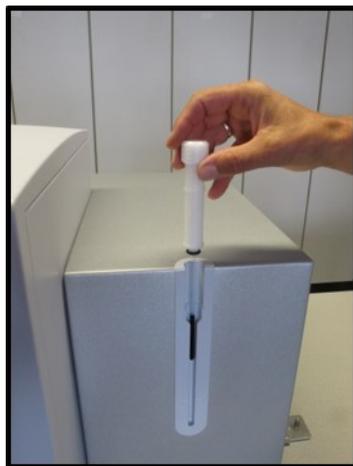


Insert the sample until it is submerged in the sample holder.

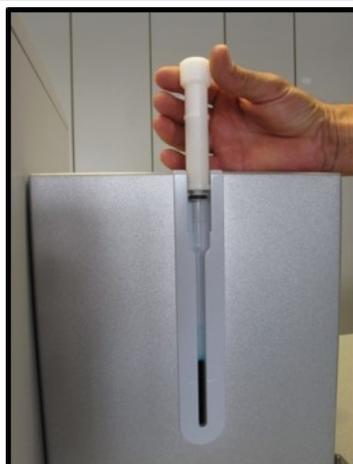


Continue to gently pull the sample down until a slight resistance is felt. Do not go too far, as this may push the cap out so that it hangs in the spinner.

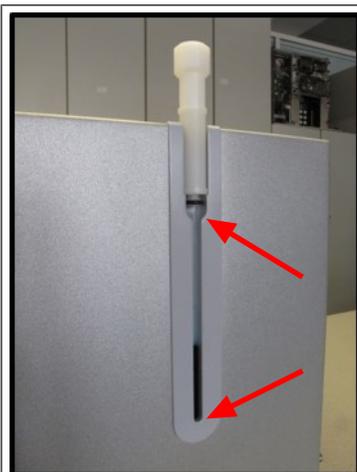
Note: Make sure your hands are clean and dry, and grasp the sample tube above the sample level to prevent contamination of the tube.



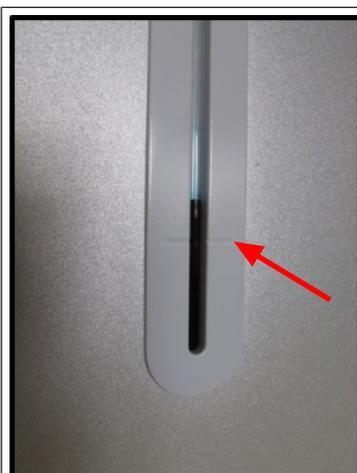
Carefully guide the sample holder and sample from above into the sample gauge on the housing.



Slowly guide the sample holder into the housing.



Guide the sample holder to the stop in the sample gauge, the sample should now be resting on the bottom of the sample gauge.



Note that the sample should be filled at least to the graduation mark.



Note on labels: 7 in. tubes can be used with standard caps that are delivered with the tubes, or so-called coded caps, as used in automation. Due to the position of the RF coil inside the magnet, almost the complete length of the tube is needed to place the sample correctly. There is only 6 mm left below the cap to place a label. Using larger labels can result in tubes which can no longer be fully inserted.

6.2.2 Temperature Stabilization and First Shimming of the System

- Put in the shim sample (5% H₂O in D₂O + 0.06mM GdCl₃).
- Enter **bringup** in the TopSpin command line.
- A window will pop up asking if the shim sample is inserted into the magnet. If so, click **OK**. If not, please put in the shim sample and click **OK**.

The system will start to acquire spectra at a large spectrum width to find the resonance line of the shim sample. It will follow the frequency offset of that resonance line from the spectrometer base frequency as set in the factory. The offset is displayed in a dialog window. The frequency offset is directly linked to the temperature of the magnet. Once the frequency offset from the factory frequency is smaller than 3 kHz, the system will automatically start to shim the system.

No further customer input is necessary after **bringup** has started. In the unlikely case that the **bringup** routine is not able to correctly set-up the spectrometer, or if you want to stop the routine for other reasons, enter **stop_bringup** in the TopSpin command line.

Please refer also to [Re-Shimming the Magnet \[▶ 35\]](#) which describes the re-shimming of the magnet in more detail. If the **bringup** routine was successful, one can skip that chapter.

6.2.3 Re-Shimming the Magnet

The shim values stored in the system and on the hard-disk were generated during the factory configuration. Because the Fourier 80 is in a new environment, the shim will no longer be within specifications. Therefore, a re-shim will be necessary.

If the system is newly installed, or has not been shimmed for a long time, it is recommended to use **fullshim**. This algorithm optimizes all shim currents and establishes a very good shim up to the highest shim orders. It can take up to several hours on the first installation of a system.

To re-shim the system, first put the shim sample into the Fourier 80. In the TopSpin command line type **fullshim** or select it from the Shim menu in the Acquisition Flow Bar sub-menu in the Manage tab. The shim routine starts and automatically optimizes the shim gradients to generate a homogeneous magnetic field at the position of the sample.

This procedure can take several hours, depending on the initial linewidth. The procedure will not stop once in specification but will keep on trying to improve the shim. It is recommended to let it run overnight.

The result of the shim routine can be checked by evaluation of the resonance line of the shim sample. To do so double click on the Acquisition Information field in the Acquisition Status Bar. The FID window of the running shim routine opens. Type `rep 990` into the command line to display the actual spectrum of the shim. Type **humpcal** in the command line. This can be done while the shim routine is still running. The command **humpcal** analyzes the lineshape of the resonance line in the spectrum window and as a result displays the linewidth at 50% and 0.55% of the maximum signal height. Note that the shim sample is a fast-relaxing sample with added relaxation agent in order to speed up the algorithm. This artificial shortening of the relaxation time of the shim sample leads to a broader line than in normal sample without added relaxation agents. If the linewidth of the shim sample approaches 1 Hz @ 50% and 24 Hz @ 0.55%, the homogeneity is well within specification (< 0.5 Hz @ 50% and < 20 Hz @ 0.55% on the lineshape sample).

The shim routine can be stopped at any time with the command **haltshim**. It will store the best shim file it generated during the run.

If the system is not used over a longer time, e.g., overnight or weekend, it is always a good practice to put the shim sample in and run **fullshim**. The magnet homogeneity can be kept at an optimum this way.

6.3 Re-Configuring a Fourier 80

In case, the configuration of a Fourier 80 needs to be updated, **cf** must be run from the TopSpin command line. This is only needed in case the magnet frequency doesn't fit the system any longer. The lock system will detect such a situation and will ask you to re-configure TopSpin.

6.4 Shimming the Sample in Daily Use

To reach a high homogeneity of the magnetic field, a shim routine has been implemented, which searches for the optimal shim by systematically adjusting the various shim gradients of the electrical shim system, while running a simple one-pulse excitation in a pseudo-2D loop.

Because this algorithm does a stepwise optimization, it typically takes longer than a gradient based shim routine. In order to speed up the shim routine, it is recommended to use the shim sample which is provided with the Fourier 80 system. This sample (5% H₂O in D₂O) gives a single resonance line with a good S/N ratio and has a reasonable fast relaxation time.

6.4.1 Shimming on the Default Shim Sample

The homogeneity of the magnetic field of a permanent magnet depends very strongly on the temperature profile of the magnet. Because small drifts in the magnet temperature and spatial temperature distribution cannot be completely avoided, the shim may slightly drift over time. **quickshim** is used on a daily basis. The algorithm results in a good shim in less than 15 minutes and relies on a good basic shim which was established using **fullshim**. In a laboratory with a stable temperature, a re-shim will not be needed more than once a day. To start the quick shim routine, either type **quickshim** in the TopSpin command line or select it from the Shim menu in the Acquisition Flow Bar sub-menu in the Manage tab.

To stop the shim routine, either type **haltshim** in the TopSpin command line or select it from the Shim menu in the Acquisition Flow Bar. The shim algorithm stores information about the best shim it could achieve and re-loads that shim set after it has been stopped. Therefore, the shim routine can be stopped at any time.

The **haltshim** command acquires a spectrum after the shim procedure has finished in order to calculate the lineshape and the S/N ratio of the shim sample. The results are stored in a log file. It is also possible to stop the shim algorithm using the command **stopshim**. In this case, no additional spectrum is acquired and no information about the shim result is stored. It is recommended to use **haltshim** because the information stored about the shim result and S/N ratio of the Shim Sample can be helpful for debugging in case of problems with the system.

Once the system is shimmed, there is no shimming necessary for individual samples. The shim will be good for several hours up to several days depending on the stability of the environment and the requirements on shim quality. Please note that the lineshapes in the spectra depend also on the natural linewidth of the samples under investigation.

6.4.2 Shimming on Other Samples

While it is recommended to shim the magnet using the standard shim sample, it is also possible to shim with your own sample. This can give a better result for some samples with a larger magnetic susceptibility.

When shimming with your own sample, use the expert mode of the shim algorithm. The Expert mode requires to create a dataset which generates a 1D spectrum of your sample of acceptable quality. The main point is that the relaxation delay d1 in the dataset is set to about 5 * T1 of the sample. T1 being the relaxation time of the sample. If the relaxation time is very long, d1 can be set to a shorter time. In this case a shorter the pulse width p1 should be used (e.g. 30%). Start **shimfourier -e -t <tunefile>** with this data set open. The shim algorithm will use the parameters from the data set and use the tune file which is given as an option in the command. Common tunefiles are `fourier_fullshim` and `fourier_quickshim`.



Depending on T1 of the sample, the shim algorithm may take considerably longer than using the default shim sample.

6.5 Locking the System

The Fourier 80 uses an external lock sample. This has several beneficial implications. First, no deuterated solvent is needed in the sample. Second, once the system is locked, it is always locked even when no sample is inserted. It also doesn't need to be re-locked when inserting a new sample, making the workflow easier and faster.

The external lock also has one drawback. Because the lock coil is at the side of the main RF coil, the field at the position of the lock coil can be slightly different from that at the position of the main coil. One effect which influences the field at the position of the lock coil is the magnetic susceptibility of the sample. Therefore, depending on the sample, small shifts of the spectra acquired can occur. They are typically very small and can be corrected for by setting the spectrum reference (parameter `sr` in TopSpin or interactively in the Process Bar).

To start the lock, type **lock** into the command line. A list will show up which allows to choose the solvent of the sample. Note that the information about the solvent is not necessary for establishing the lock because the lock uses an external unchangeable sample. But the information about the solvent is stored in the dataset. If the system is already locked, it will not be re-locked and will only transfer the solvent information to the newly acquired datasets.

As mentioned above, when changing samples, a new lock command is not necessary.

The lock automatically starts at system startup.

The lock can be monitored in the BSMS display.

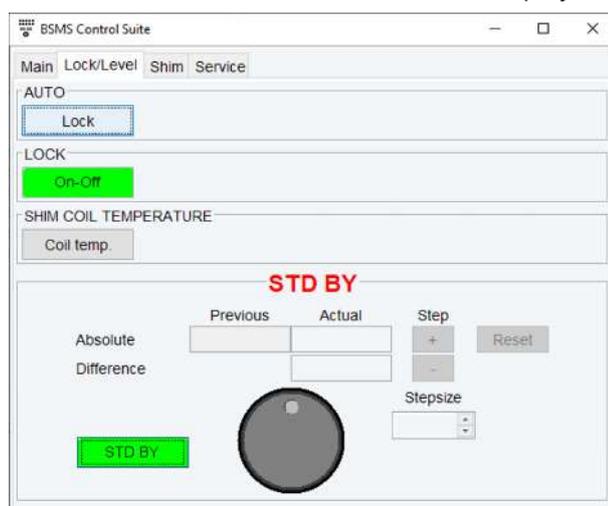


Figure 6.2: The BSMS Control Suite

The green **LOCK On-Off** button in the Lock menu of the BSMS Control Suite indicates that the system is properly locked. If the system is not locked or the lock is not stable, this button turns to red. Please note that this is typically the case when the shim algorithm is running because the changing shim gradients also influence the lock stability. Once the shimming is done, the lock will be stable again.

The **LOCK On-Off** button can also be used to switch the Lock on or off.

Please note, that it may take some time before the lock is stable after switching it on and, thus, it may take some time before the **LOCK On-Off** button turns to green. The time to establish the Lock depends on the sample and the PID regulation parameters of the Lock (typically 15-20 seconds). The time for the **Lock** button to turn green is typically a bit longer because the lock algorithm checks the lock stability in a moving time window and the button turns green if the lock regulation is fully within pre-defined limits over that time window.

If the acquisition status bar is open, the lock status can also be checked in the BSMS status indicator. The following screenshot shows a stable lock.



Figure 6.3: The BSMS Status Message

6.6 Monitoring the Magnet and Shim Temperature

The temperature stability of the magnet and the shim system is of major importance for the stability of the Fourier system. Both temperatures are automatically controlled and regulated once the system is switched ON. If the acquisition status bar is open, the magnet and shim system temperature can be monitored.

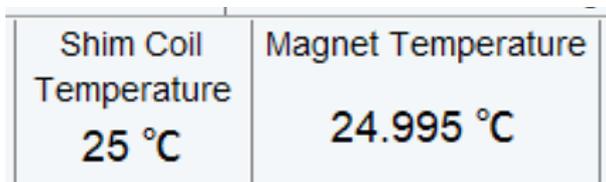


Figure 6.4: Temperature Display for Magnet and Shim Coil

Both temperatures should be at 25 °C. The magnet temperature is stable if it is within a range of +/- 5 mK. If one of the temperatures was outside of its stability limits within a moving time window, the display goes from black to red.

6.7 Measuring the Sample

The individual steps of a measurement depend on the specific NMR application or context of the measurement, this section contains basic steps in general.

NOTICE

Danger from improper handling

- ▶ The system is only intended for indoor use!
- ▶ Pay attention that no sample material falls into the magnet!
In case sample material has fallen into the magnet, do not perform measurements and, if necessary, stop the current measurement. In this context observe applicable standards for contamination. The system comes with a cleaning kit which allows the user to remove a broken sample tube and spilled out sample from the probe. In case of doubt or if help is needed, contact the Bruker Service.

⚠ CAUTION



Risk of injury or material damage from broken glass/sample tubes

Improper handling of the sample tubes may result in material damage and personal injury caused by glass fragments.

- ▶ Handle the sample tubes carefully, because they are fragile and can easily break.
- ▶ Insert and remove the sample tubes with utmost caution.

Preparing the measurement

- Insert the sample tube.
- Wait some seconds for the lock to be stable again.

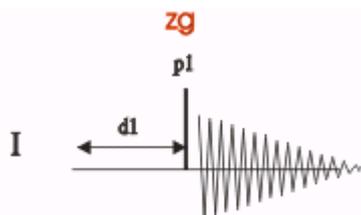
As an example, the acquisition of a 1D proton spectrum is explained below.

6.7.1 First Proton Spectrum

This chapter describes the acquisition and processing of a one-dimensional ^1H NMR spectrum of the Shim Sample using the Fourier parameter set **PROTON_f**. This experiment can be also be used to check the basic function of a newly installed Fourier 80 spectrometer.

For the first Proton spectrum on the Fourier, the shim sample which is delivered with the system can be used. The following description is based on that sample (e.g. solvent is D_2O).

The pulse sequence **zg** (see figure below) consists of the recycle delay, the radio-frequency (RF) pulse, and the acquisition time during which the signal is recorded. The two parameters, **d1** and **p1**, correspond to the length of the recycle delay and the length of the 90° RF pulse, respectively.



The time intervals depicted in the pulse sequence diagrams are not drawn to scale. For example, **d1** is typically a few seconds while **p1** is typically a few microseconds in length.

6.7.1.1 Experiment Setup

Create a new dataset

- On the menu bar, click **Acquire | Create Dataset** to open the Create New Dataset window.

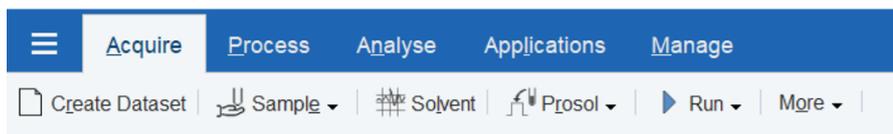


Figure 6.5: Acquisition Flow Bar

- In the Create New Dataset window, enter or select:
 NAME = **Proton_exp** (this is just an example name, you can use any name)
 EXPNO = 1
 Directory = e.g. C:\Data

Figure 6.6: Create a New Dataset

Directory, **NAME** and **EXPNO** define where the new experiment dataset will be stored on the computer:



Directory/NAME/EXPNO/ In the example: C:\Data\proton_exp\1

Directory can be selected in the drop-down list, or a new location can be typed in the text field. **NAME** is a subdirectory of **Directory**, and **EXPNO** is a subdirectory of **NAME**. **EXPNO** must be a positive integer. It provides a way to store multiple related datasets under the same **NAME**.

- In the Parameters group  Parameters click **Read parameterset** and **Select** to open the rpar window.

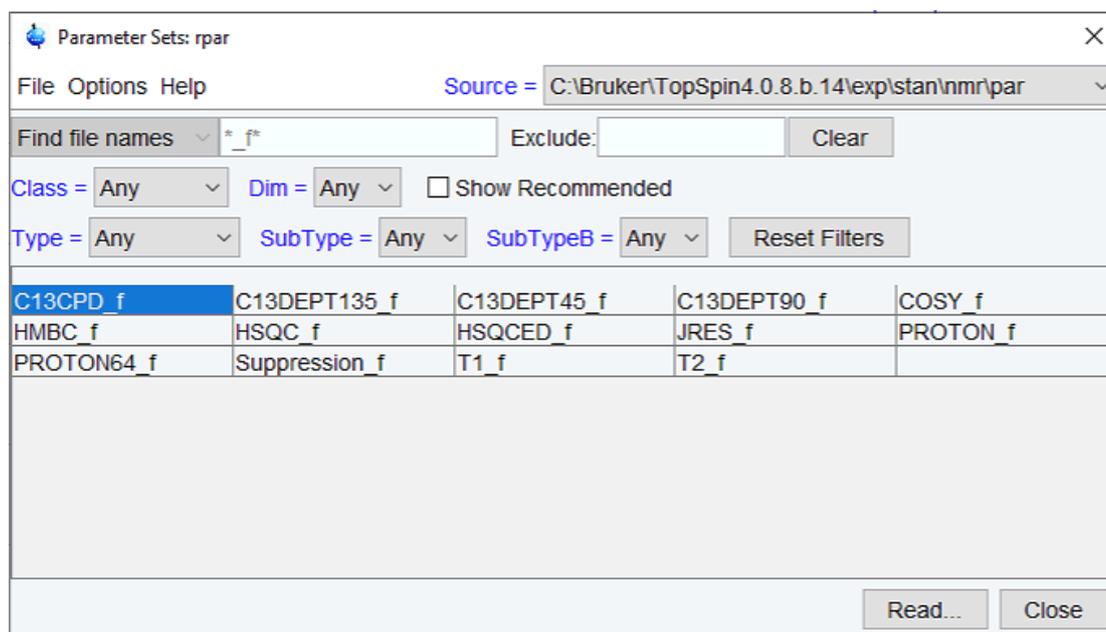


Figure 6.7: Parameter Sets - rpar

- Ensure that the source directory is
 <Topspin>\exp\stan\nmr\par
 and not
 <Topspin>\exp\stan\nmr\par\user
- In the table select **PROTON_f** as experiment and click **Set selected item in editor**.
- In the Create New Dataset window check **Set solvent** and in the drop-down list select **D2O** (for the shim sample).
- In the TITLE field enter a text stating the experiment, sample, the solvent and any other useful information. The title information can be used to search for a dataset.
- In the New Dataset window, click **OK**.

To acquire a spectrum, use the Workflow buttons in the Acquisition bar from left to right (see steps below). Alternatively, commands which are displayed in brackets of the various popup windows, can also be typed at the TopSpin command prompt (e.g. **lock**).

Load the sample

- In case there is no sample changer, the **Sample** tab is not used.
- Put the shim sample in the sample holder and adjust the correct sample depth with the depth gauge on the front of the electronic housing.
- Insert the sample into the magnet. Be careful not to put any lateral forces on the sample tube as it can easily break. Push it down gently, the sample tube should easily slide into the magnet bore.



The sample is completely in if only the slightly thicker upper part of the sample holder is still visible.

Choose the solvent

The Fourier 80 system uses a permanently installed external lock sample. Therefore, the system stays locked in normal operating conditions. No lock command is required.

But the information about the solvent is written into the dataset for reference. If not done already when creating the data set, it can be done at any time using the **Solvent** tab.

Solvent	Description
Acetic	acetic acid-d4
Acetone	acetone-d6
C6D6	benzene-d6
CD2Cl2	dichloromethane-d2
CD3CN	acetonitrile-d3
CD3CN_SPE	LC-SPE Solvent (Acetonitrile)
CD3OD_SPE	LC-SPE Solvent (Methanol-d4)
CDCl3	chloroform-d
CH3CN+D2O	HPLC Solvent (Acetonitril/D2O)
CH3OH+D2O	HPLC Solvent (Methanol/D2O)
D2O	deuteriumoxide
D2O_salt	deuteriumoxide with salt
Dioxane	dioxane-d8
DMF	N,N-dimethylformamide-d7
DMSO	dimethylsulfoxide-d6
EtOH	ethanol-d6
H2O+D2O	90%H2O and 10%D2O
H2O+D2O_salt	90%H2O and 10%D2O with salt
HDMSO	90%DMSO and 10%DMSO-d6
Juice	fruit juice
MeOD	methanol-d4
Plasma	blood plasma
Pyr	pyridine-d5
T_H2O+D2O+Me4NCI	(CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer
T_H2O+D2O+NaAc	sodium acetate in 90%H2O and 10%D2O, for NMR thermometer
T_H2O+D2O+Pivalate	pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer
T_MeOD	methanol-d4, for NMR thermometer
TFE	trifluoroethanol-d3
THF	tetrahydrofuran-d8
Tol	toluene-d8
Urine	urine

Lock nucleus: 2H [v] [OK] [Cancel]

Figure 6.8: Solvents Table

Load the Prosol parameters

- On the Workflow button bar, click **Prosol**.

This will load calibrated pulse lengths and power levels according to the definitions in the parameter set.

6.7.1.2 Acquisition

Start the data acquisition

- On the Workflow button bar, click **Run**.
- or
- On the **Run** button, click the **drop-down** arrow to see more options.

6.7.1.3 Processing

- When the acquisition has finished, click **Process** on the menu bar.
- On the **Proc Spectrum** button, click the **drop-down** arrow to see more options.
- In the list, select **Configure Standard Processing (proc1d)**.
- In the proc1d window, enable the following options:
 - Exponential Multiply (em)
 - Auto - Phasing (apk)
 - Auto - Baseline Correction (absn)

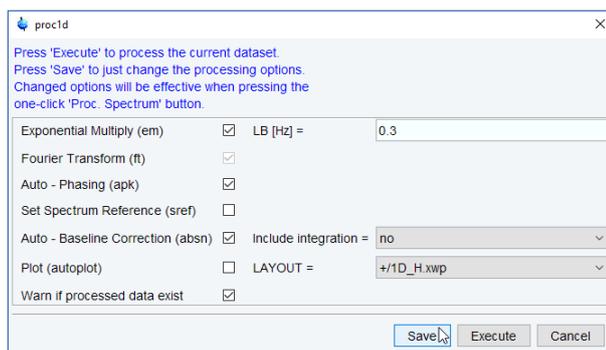


Figure 6.9: Processing Options

- If TMS is added to the sample for referencing, enable **Set Spectrum Reference (sref)**.
- In the proc1d window, click **Execute** and then click **Save** to save the selected processing settings.

Now all future datasets can be processed with the defined actions with a click on **Proc Spectrum**.

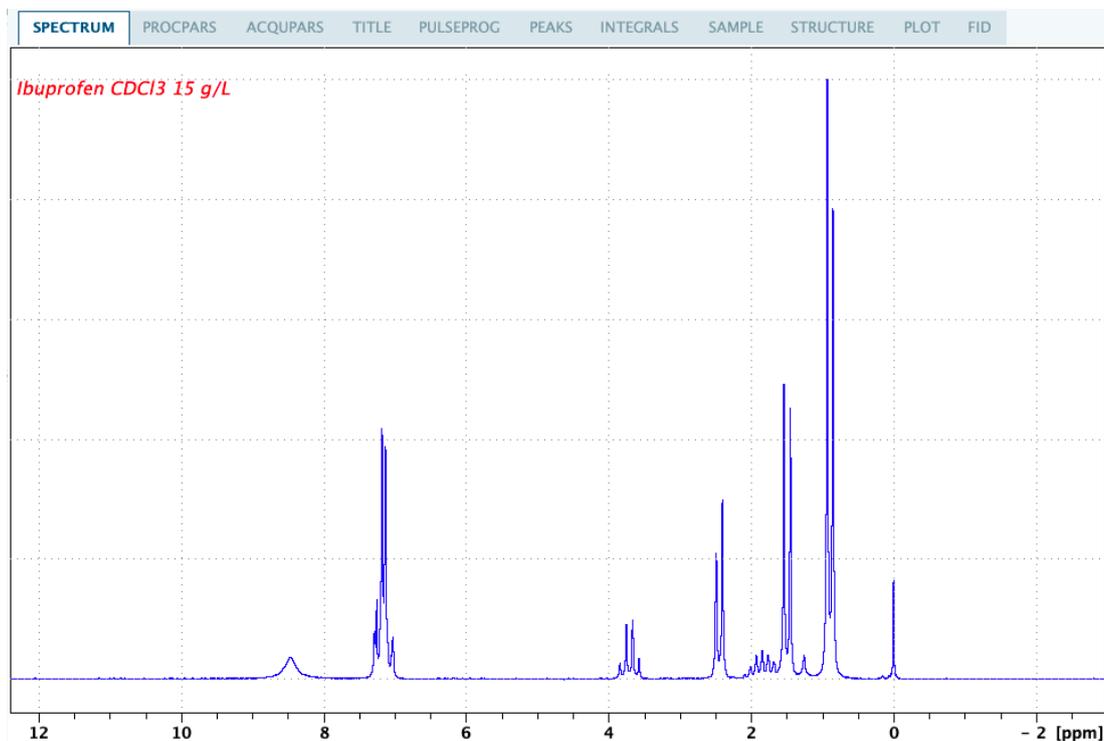


Figure 6.10: Spectrum Example

6.8 Turning the Spectrometer Off

The power switch is located on the back panel of the spectrometer. Pressing the switch turns the spectrometer off. The status LED on the front turns off indicating that the system has been shut down.

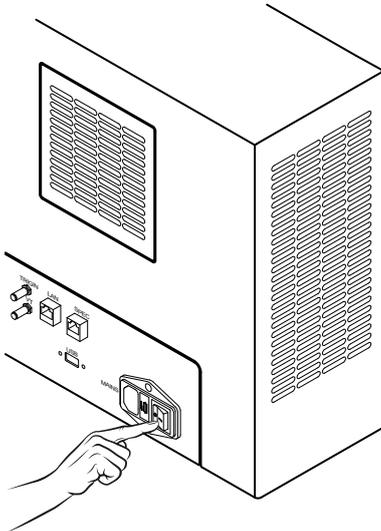


Figure 6.11: Location of the Power Switch

7 Maintenance

The Fourier 80 is a low-maintenance spectrometer. Only perform maintenance procedures described in this section. Maintenance procedures not described herein may only be performed by authorized personal and/or the Bruker Service.

Bruker does not incur any liability in case of infringements!

WARNING

Exposure and other health hazards to maintenance personnel.

If contaminated, the device must be cleaned before any maintenance work can be performed.

- ▶ Register all substances with which the device has come into contact.
- ▶ Sign a certification form verifying that the device has been properly cleaned if contaminated to protect maintenance personnel.
- ▶ Obviously contaminated, insufficiently cleaned units, as well as units without a signed cleaning certification will not be repaired and will be returned to the sender.



7.1 Cleaning the System

- Clean the system's housing only by using a dry or damp tissue.
- Do not use cleansing agents which include organic solvents, acids or bases.
- Prevent any particulates from entering the system.
- The filters of the system should be checked once a year. If they need cleaning depends on the environment and the working hours of the system.

7.2 Replacing the Filter on the Back Side



Filter grill on the back of the electronics unit above the connection panel.



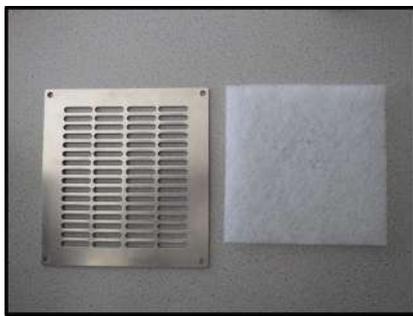
Remove the four screws using a TX20 Torx key.



Remove the filter grill.



Remove the old filter.

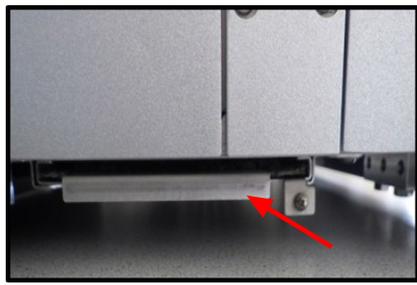


Insert a new filter P/N H176516.

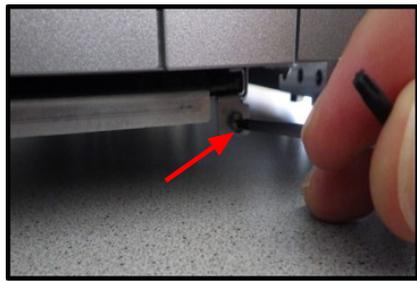


Tighten the four screws using a TX20 Torx key.

7.3 Replacing the Bottom Filter



Bottom Filter Housing (P/N H176414) with filter drawer on the bottom front electronic unit.

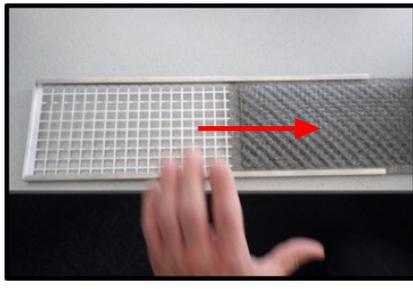


Loosen the screw using a TX10 Torx key.

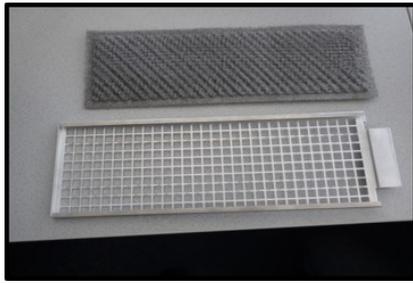


Remove the filter drawer.

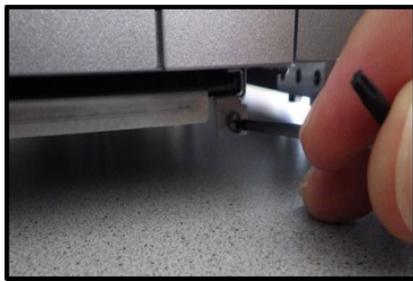




Pull the metal filter out of the guide.



Clean the metal filter with compressed air or replace it with a new one (H176405 F80 HOUSING WIRE FILTER MATTE).



Insert the filter and drawer in the unit. Secure the drawer with the screw.

8 Troubleshooting

This chapter describes possible problems relating to the system's hardware components, their potential causes and recommended solutions. If the recommended solutions do not solve the problem, contact the Bruker Service Hotline.

For problems relating to the user software refer to the corresponding help of your software application.

Problem: Status LED does not light

Cause	Solution
The spectrometer is not/not correctly connected to the main supply.	<ul style="list-style-type: none"> • Check the connection to main supply. • If necessary, connect the spectrometer as described in Connecting to the Mains Supply [▶ 30].
The spectrometer is turned off.	<ul style="list-style-type: none"> • Turn the spectrometer on as described in Starting the Fourier 80 [▶ 31].

Problem: Sample/sample rest in the magnet opening

Cause	Solution
A sample or sample rest has fallen in the magnet's opening.	<ul style="list-style-type: none"> • Do not perform a measurement or stop the current measurement. • Use the cleaning kit provided with the system to remove any sample and glass from the probe (see instructions provided with the cleaning kit). • In case, you don't want to clean it yourself or if you need help with the cleaning process, contact the Bruker Service Desk.

Problem: Sample cannot be analyzed

Cause	Solution
A sample cannot be analyzed due to a too large sample label.	<ul style="list-style-type: none"> • Remove the sample label before analysis.

Problem: Bad spectrum or artifacts

Cause	Solution
External interference.	<ul style="list-style-type: none"> • Avoid installation or operation of interfering devices (see Site Planning [▶ 23]).
Insufficient homogeneity of field.	<ul style="list-style-type: none"> • Start shim routine on Shim Sample.

9 Replacement of Parts



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 warranty.

Loss of Guarantee

The use of non-approved spare parts will invalidate the manufacturer's warranty.

Purchase spare parts from authorized dealers or directly from the manufacturer. See Contact for manufacturer's address.

9.1 Spare Parts List

Part Number	Description	Comment
Z10688	Shim Sample	Reference sample
Z10689	Lineshape Sample	Reference sample
180717	5 x 20 mm 6.3 A T Fuse	See Replacing the Fuse [51]
H176415	Fourier 80 Accessories Case	
H176416	Fourier 80 USB Stick (software)	
H176417	Fourier 80 Cleaning Kit	

Table 9.1: Spare Parts

9.2 Replacing the Fuse

The Fourier 80 uses a 5 x 20 mm 6.3 A T fuse (P/N 180717).

WARNING

Risk to life from electrical shock

A life-threatening shock may result when the housing is open during operation.

- ▶ Only qualified personnel should open the housing.
- ▶ Disconnect the device from the electrical power supply before opening the device. Use a voltmeter to verify that the device is not under power!
- ▶ Be sure that the power supply cannot be reconnected without notice.



Replacement of Parts



Set mains switch to zero, then unplug the power cord.



Pull out the middle slot.



Take the fuses out of the holder.



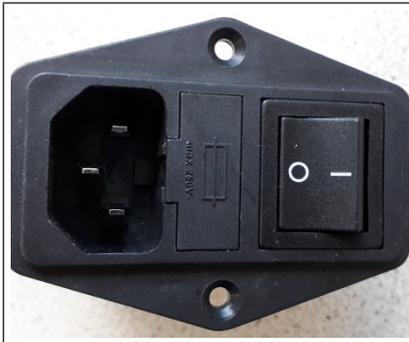
Replacement fuses P/N 1801717.



Insert fuse in the slot.



Slide the drawer back into the middle bay provided for this purpose.



Insert until it is flush again.



Reconnect the mains plug and set the mains switch back to position 1.

9.3 Returning the Unit for Repair

If the Bruker Hotline diagnoses an instrument failure that requires a part to be returned for repair, please follow the procedure listed here:

1. Contact your local Bruker office to start the repair process (see Contact). Repair is always handled by your local Bruker office. Their reply will contain all necessary information for the subsequent repair process steps.
2. They will provide you with details on the shipping address, and also in most cases a “Return Merchandise Authorization” number (RMA number) that allows references to the repair case. Always refer to this RMA number in case of questions.
3. Send the defective part to the local Bruker office and include the following documents:
 - RMA sheet (if RMA number was assigned).
 - Signed Equipment Clearance Form (BBIOF002/H152631). The Equipment Clearance Form will be sent to you as part of step 1 (see above) with information about the returned part (part number, serial number, your contact details) already filled in.
4. Attach the relevant papers to the *outside* of the packaging, for instance in a transparent polybag.



The unit should be returned using the original container and packing assembly. If this packaging is no longer available, contact your local Bruker office for further instructions.

10 Dismantling and Disposal

Following the end of its operational life, the devices must be dismantled and disposed of in accordance with the 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 warranty.

10.1 Dismantling

Before starting dismantling:

1. Shut down the device and secure to prevent restarting.
2. Disconnect the power supply from the device.
3. Remove consumables, auxiliary materials and other processing materials and dispose of them 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.

10.2 Disposal in Europe

Environmental information for laboratory and industrial customers within the EU (European Union)



This laboratory product is developed and marketed for Business-to-Business (B2B), so does not fall under article 6 clause 3 of the German Act ElectroG. To meet the demands of the European Directive 2012/19/EU WEEE 2 (Waste of Electrical and Electronic Equipment) and the national Equipment Safety Act, electrical and electronic equipment that is marked with this symbol directly on or with the equipment and/or its packaging must not be disposed of together with unsorted municipal waste or at local municipal waste collecting points. The symbol indicates that the equipment should be disposed of separately from regular industrial/domestic waste.

Correct disposal and recycling will help prevent potential negative consequences for the environment and risk to personal health. It is your responsibility to dispose of this equipment using only legally prescribed methods of disposal and at collection points defined by government or local authorities in your area.

The WEEE register number can be found on the product label of the equipment. If you need further information on the disposal of equipment or collection and recovery programs available, contact your local Bruker BioSpin sales representative. Local authorities or professional waste management companies may also provide information on specific waste disposal services available in your area.

Disposal - End of Life (EoL) information

After the lifespan of an electrical and electronic product, Bruker BioSpin takes responsibility for final disassembly and correct disposal in accordance with the European directive WEEE 2012/19/EU.

Bruker BioSpin offers to take back the equipment (only for deliveries after 23.03.2006) after termination of use at the customer site upon request by the customer. Additional costs for dismantling and transport service will apply!

Only 100% pre-decontaminated equipment can and will be accepted by Bruker BioSpin. A release document for decontamination (Equipment Clearance Form) can be requested from your nearest Bruker BioSpin contact site, following the Return Material Acceptance (RMA) process when repairs, going back to Bruker sites, are requested.

In compliance with WEEE II directive: **2012/19/EU**

10.3 Disposal in USA and Other (non-EU) Countries

Disposal of these materials may be regulated due to environmental considerations. For disposal or recycling information, please contact our local office or your local authorities, or in the U.S.A., contact the Electronics Industry Alliance web site at www.eiae.org.

11 Technical Data

11.1 Drawings

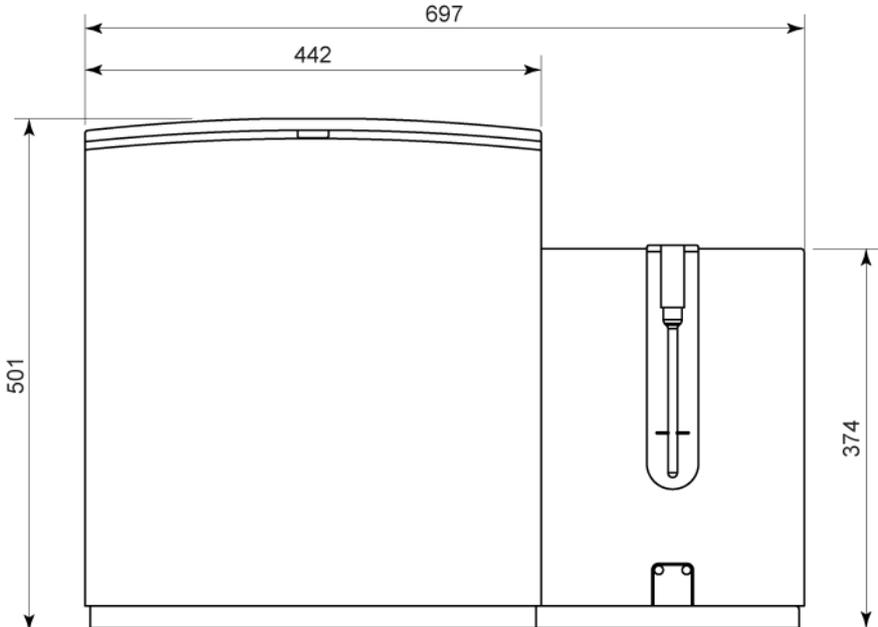


Figure 11.1: Drawing — Front View (all dimensions in mm)

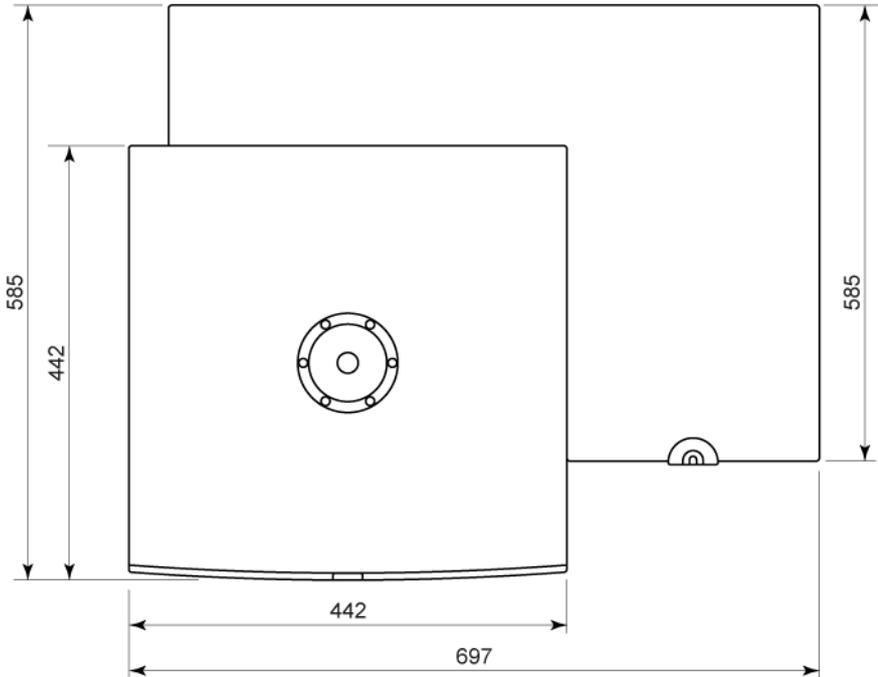


Figure 11.2: Drawing — Top View (all dimensions in mm)

11.2 Specifications

In this chapter only hardware-related specifications are listed. For further information concerning the user software refer to the corresponding Online Help of the software application used by you.

11.2.1 General

Parameter	Value/Definition
Dimension (L x W x H)	59 x 70 x 51 cm
Weight*	94 - 96 kg

* The weight varies depending on the used accessories or options.

11.2.2 Connection Values

Parameter	Value/Definition
Electrical	
Voltage	110-230 V
Apparent power consumption	Maximum 500 VA
Frequency	50/60 Hz
Circuit protection AC	2 x 6.3 A / 250 V / slow-blow fuses

11.2.3 Ambient and Operating Condition

Parameter	Value/Definition
Operating altitude	Maximum 2000 m ASL (a.s.l.)
Temperature range	18 - 28 °C Optimal: 22 - 25 °C
Humidity range (non-condensing)	20 - 80%
Relative humidity	<ul style="list-style-type: none"> • Maximum 80% for temperatures up to 31 °C, or • Decreasing linearly to 50% at 40 °C
Mains supply voltage fluctuations	Up to $\pm 10\%$ of the nominal voltage
Transient overvoltage	Up to the level of <i>Overvoltage Category II</i>
Pollution degree	2
Protection class	IP20
Safety requirements for electrical equipment for measurement, control, and laboratory use – Part 1: General requirements	<ul style="list-style-type: none"> • EN 61010-1:2010 (IEC 61010-1:2010 + Cor. :2011) • ANSI/UL 61010-1:2012-05-11 • CAN/CSA-C22.2 No. 61010-1-12

11.3 Rating Plate

The system's rating plate is located on its rear side.



Figure 11.3: Rating Plate Sample

1	Registration number of WEEE guideline (Waste of Electrical and Electronic Equipment)	5	Product number (PN)
2	Voltage and apparent power consumption	6	Serial number (SN)
3	Specifications for the fuses used	7	Engineering Change Level (ECL)
4	Order number		

12 Contact

Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany

E-Mail: nmr-support@bruker.com

<http://www.bruker.com>

WEEE DE43181702

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:

<https://www.bruker.com/service/information-communication/helpdesk.html>

 **Bruker Corporation**

info@bruker.com
www.bruker.com



Order No: H172348

Specifications for benchtop NMR

1.0 Background and Justification

The US EPA's Office of Research and Development (ORD) through the National Research Programs has the responsibility of developing and applying state-of-the-art methods, measurements, models, and tools to complex environmental issues. The need to quickly and accurately identify the toxicity from emerging contaminants is a major requirement of many EPA research programs.

Analytical quality control (AQC) is beneficial for sample testing such as high throughput bioactivity assays. AQC characterizes chemical identity, purity, concentration, and stability for such samples. Multiple kinds of instrumentation have been considered and applied previously for AQC work, specifically during the Tox21 project which, over multiple years, applied Liquid Chromatography Mass Spectrometry (LC-MS), Gas Chromatography Mass Spectrometry (GC-MS), and Nuclear Magnetic Resonance (NMR) to tens of thousands of samples associated with ~8000 chemicals. Unlike other techniques, NMR has only one major issue in regard to amenability to detection – whether or not a chemical has one or more magnetically active nuclei (that are not in dynamic exchange) but this constraint is not an issue for the majority of chemicals because most contain protons, carbons or fluorine which are all detectable. NMR can supply information on all three characteristics of chemical identity, purity, and concentration without the challenges associated with calibration for other approaches such as mass spectrometry. This will allow tens to hundreds of sample analyses per week with minimal operator input. Such instrumentation and throughput will allow CTE to confirm chemical identity, as well as report the concentration and purity of target compound(s) in the sample for the ER/AR project, samples in the ToxCast/Tox21 library, as well as future needs including ^{19}F NMR to support PFAS analysis.

2.0 Specifications and Requirements for Benchtop NMR

Benchtop instrument ($\geq 80\text{MHz}$) which operates at room temperature without cryogenic liquids

Computer (with peripherals) and software needed to acquire and process data

Autosampler with space for at least 50 sample tubes and ability to array multiple experiments for multiple samples

Sensitivity to measure ^1H NMR for 20 mM samples in ≤ 10 minutes

^1H , ^{13}C and ^{19}F multinuclear probe capable of 1D and 2D NMR including, at minimum, 1D multiplicity detection, homonuclear 2D ^1H - ^1H and ^{19}F - ^{19}F detection, and heteronuclear 2D ^1H - ^{13}C one-bond and long-range detection experiments

Achievable resolution based on ^1H standard sample (at 50/0.55/ 0.11% signal height): $\leq 0.5/ 15/ 30$ Hz

Achievable ^1H sensitivity (on multinuclear probe) based on 1% ethylbenzene: $>110:1$

File format compatible with ACD/Labs Spectrus Software

Capable of providing data to assess compound identification, purity, and concentration from a single analysis

Instrument familiarization and application specific on-site training.

Instrument maintenance and user's manuals

110V, 60 Hz power; UL (or equivalent) rated

1 year manufacturer's warranty included; four 1-year option periods for basic maintenance and service agreement

Commercial-off-the-shelf availability